

Majoron-Emitting Double Beta Decays in the LUX-ZEPLIN (LZ) Experiment

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Doctor of Philosophy

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Statement of Originality

I hereby declare that the content of this thesis represents a collection of my original work. Any work from others is either referenced appropriately, or indicated clearly in text in the case of work under development with no available public information. A summary of my specific contributions in each chapter is provided as below.

Chapter 1 describes the theoretical background and motivation of the search for Majoron-emitting double beta decay. This is followed by an overview of the main experimental technologies to search for the process.

Chapter 2 introduces the underlying scintillation and ionisation mechanisms in liquid xenon and how they apply to the principle of operation of a dual-phase xenon time projection chamber. The chapter then focuses on the detector design and subsystems of the LZ experiment.

Chapter 3 presents the projected sensitivity of the LZ experiment to $n = 1, 2, 3, 7$ modes of Majoron-emitting double beta decay. The analysis is all my own work, utilising the simulations and statistical tools developed within the LZ Collaboration.

Chapter 4 studies the effect of spatial non-uniformity of radon progeny as observed in the LZ detector. The work builds on the radon progeny identification framework by Nicolas Angelides at Imperial College London, and the ion fraction study by Emily Perry at University College London, both are members of the LZ collaboration. My individual contribution is the development of a novel ^{214}Pb tagging method based on decay branching ratio, and the impact of ^{214}Pb spatial distribution on the sensitivity of the LZ experiment to ^{136}Xe Majoron-emitting double beta decay.

Chapter 5 focuses on the search for ^{136}Xe Majoron-emitting double beta decay using a data set obtained in the LZ experiment. The energy resolution determination builds on the work by Guilherme Pereira at LIP - Laboratório de Instrumentação e Física Experimental de Partículas, Coimbra, as published in Ref. [1]. The activity determination of each component in the background model follows results published by the LZ Collaboration in Ref. [2]. The activity scaling factors of detector components are obtained by my analysis that builds on work by Aiham Al Musalhi at University of Oxford. My individual contributions include adapting the activity determination work to Majoron-emitting double beta decay, building the background model and all of the subsequent data analyses.

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Abstract

The scale of neutrino masses is distinct from that of other particles, hinting towards an alternative mass generation mechanism beyond the Standard Model. One promising approach is to consider neutrinos acquiring Majorana masses through spontaneous symmetry breaking of the global $U(1)_{B-L}$ symmetry, with the corresponding Goldstone boson denoted as the Majoron. The particle can potentially be discovered via the hypothetical Majoron-emitting double beta decay ($0\nu\beta\beta\phi$). Observing such a process would illuminate numerous physics searches, including neutrino mass generation, leptogenesis of matter-antimatter asymmetry, and potential candidates for dark matter particles.

In this thesis, the capability of the LUX-ZEPLIN (LZ) experiment to search for $0\nu\beta\beta\phi$ in ^{136}Xe is demonstrated. For the most commonly searched $n = 1$ mode, a conservative lifespan of 500 live-days will enable LZ to exclude $T_{1/2} < 4.75 \times 10^{23}$ yr at 90% CL. The $T_{1/2}$ sensitivities to $n = 2, 3, 7$ modes are also studied, showing that LZ will likely reach competitive results against the current best limits. As a validation, the LZ SR1 $0\nu\beta\beta\phi$ background model constrains the half-life of the $2\nu\beta\beta$ decay of ^{136}Xe to $T_{1/2} = 2.25 \pm 0.22 \times 10^{21}$ yr, in agreement with the literature value of $T_{1/2} = 2.165 \pm 0.016(\text{stat}) \pm 0.059(\text{sys}) \times 10^{21}$ yr as obtained by EXO-200 [3]. A search for the $n = 1$ $0\nu\beta\beta\phi$ mode is performed with the LZ SR1 data set, showing that LZ can set a lower limit of $T_{1/2} > 2.1 \times 10^{23}$ yr at 90% CL with an $83.4 \text{ kg} \cdot \text{yr}$ exposure of ^{136}Xe . This provides a concrete demonstration that LZ is capable of searching for ^{136}Xe $0\nu\beta\beta\phi$ and reaching competitive results in its full lifespan. It also highlights the general-purpose nature of a multi-tonne scale liquid xenon TPC and adds to the potential scientific goals of next-generation detectors.

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Introduction

The aim of this thesis is to provide a comprehensive demonstration of the potential reach of the LUX-ZEPLIN (LZ) experiment in the search for Majoron-emitting double beta decay ($0\nu\beta\beta\phi$). The organisation of the thesis is as follows:

Chapter 1 provides an overview of the theoretical background and motivation to search for $0\nu\beta\beta\phi$. The observation of neutrino oscillations is briefly introduced, followed by the concept of Majorana mass. This is then linked to the seesaw mechanism of neutrino mass generation. The Majoron is introduced as a natural consequence of $B - L$ violation, and the important physics problems it can address are discussed. The observable process, $0\nu\beta\beta\phi$, is introduced, together with the neutrinoless double beta decay ($0\nu\beta\beta$) in its standard form. A review of the Majoron models and their classifications is provided. Finally, the experimental signal and strategy to search for the process are discussed, along with an overview of the main experimental technologies that are currently active in the field.

Chapter 2 provides the necessary background to discuss the search for $0\nu\beta\beta\phi$ with the LZ experiment. The physical processes in a dual-phase liquid xenon (LXe) time projection chamber (TPC) and how they lead to primary and secondary scintillation signals are shown. The chapter then illustrates the detector systems of the LZ experiment.

Chapter 3 studies the sensitivity of the LZ experiment to $0\nu\beta\beta\phi$. The LXe and detector response to $0\nu\beta\beta\phi$ events is simulated and studied in the observable parameter space. The major background sources in the context of LZ are listed, together with their estimated rates. An optimisation method for the fiducial volume (FV) and region of interest (ROI)

for different $0\nu\beta\beta\phi$ modes is presented. Finally, the statistical framework to project half-life sensitivity is introduced, and the sensitivity estimates for various $0\nu\beta\beta\phi$ modes are compared against world-leading results to demonstrate LZ's competitiveness in the field.

Chapter 4 assesses the impact of the newly-observed spatial non-uniformity of ^{214}Pb on the ability of LZ to search for $0\nu\beta\beta\phi$. The radon decay chains are introduced, followed by the illustration of non-uniformity observed for some radon progeny. A novel tagging method of ^{214}Pb is developed, and its limitation to apply to currently available data is discussed. An alternative approach is taken to estimate the spatial distribution of ^{214}Pb , which is then used to estimate the impact on $0\nu\beta\beta\phi$ sensitivity.

Chapter 5 presents the results of a search that showcases the $n = 1$ mode of $0\nu\beta\beta\phi$ in the LZ SR1 dataset. The analysis cuts for the search are listed, and the energy resolution applicable to the dataset is determined. The background model for the search is reassessed based on real data, and the complete background model is validated by comparing the inferred half-life of a known background source to the literature value. The global fitting and statistical inference is performed, leading to the final lower limit result on the half-life of the $n = 1$ mode of $0\nu\beta\beta\phi$.

Chapter 6 summarises the key takeaways of the analysis work presented in this thesis, along with potential future work to improve the search for $0\nu\beta\beta\phi$ with LZ.

Chapter 1

Majoron-Emitting Double Beta Decay

This chapter provides an overview of the theoretical background and motivation for the search for Majoron-emitting double beta decays. The key features of some commonly studied models and the general classification of models for Majoron emission are presented. Then, the experimental signature and search strategy for the decay mode is discussed. The chapter concludes with a review of experimental technologies and their search results for Majoron emission.

1.1 Neutrino Mass

1.1.1 Neutrino Oscillations

The observation of oscillation between different neutrino flavours provides the first direct evidence of neutrino masses, hinting towards physics beyond the Standard Model [4–6]. Since neutrinos are produced in definite flavour eigenstates via the weak interaction, they should remain in their original flavours indefinitely if massless. However, if neutrinos have definite mass eigenstates with eigenvalues m_i , each state will evolve as $|\nu_i(t)\rangle = e^{-ip \cdot x} |\nu_i(0)\rangle$, where p and x are the momentum and position four-vectors. This introduces phase differences between different mass eigenstates under the same propagation distance, provided that the eigenvalues are non-degenerate. In addition, a flavour eigenstate $|\nu_\alpha\rangle$ can be decomposed into a linear superposition of mass eigenstates $|\nu_i\rangle$ through the unitary Pontecorvo-Maki-

Nakagawa-Sakata (PMNS) matrix $U_{\alpha i}$. In the ultra-relativistic limit, one can arrive at the following oscillation probability [7]:

$$\begin{aligned}
P(\nu_\alpha \rightarrow \nu_\beta) &= |\langle \nu_\beta(t) | \nu_\alpha \rangle|^2 \\
&\simeq \sum_i \sum_j U_{\beta i}^* U_{\alpha i} U_{\alpha j}^* U_{\beta j} e^{-i \frac{(m_i^2 - m_j^2)}{2E} x}.
\end{aligned} \tag{1.1}$$

The above expression shows that oscillation probabilities between different flavours are only dependent on the splitting between squared masses of the mass eigenstates, rather than the individual neutrino masses. On the experimental side, there are two mass splitting parameters that can be directly measured, one from solar neutrinos and the other from atmospheric neutrinos. In general neutrino formalism, the two parameters are commonly denoted as $\Delta_{21}m^2$ and $\Delta_{32}m^2$ respectively. For the purpose of consistency with referenced literature, this work adopts the notation of δm^2 for the solar parameter, and Δm^2 for the atmospheric parameter [8]. These two parameters are defined as:

$$\begin{aligned}
\delta m^2 &\equiv m_2^2 - m_1^2, \\
\Delta m^2 &\equiv m_3^2 - \frac{m_1^2 + m_2^2}{2}.
\end{aligned} \tag{1.2}$$

While not capable of revealing the exact mass eigenvalues, measurement of the sign and value of these two parameters allows one to set the ordering of mass eigenstates. Experimental data were compared against the theoretical prediction of the Mikheyev–Smirnov–Wolfenstein (MSW) effect (matter effect) [9, 10], the effect of matter with varying density on the change of flavours, and showed that $\delta m^2 > 0$ [11]. Unfortunately, a similar kind of effect is not present for Δm^2 , posing ambiguity in the sign of the parameter and leading to the famous “mass ordering problem”. The mass spectrum of which $m_1 < m_2 < m_3$ (or equivalently $\Delta m^2 > 0$) is referred to as “Normal Ordering” (NO) and the one with $m_3 < m_1 < m_2$ (or equivalently $\Delta m^2 < 0$) is “Inverse Ordering” (IO). One of the major objectives of current and next-generation neutrino experiments is to resolve this ambiguity in neutrino mass ordering via their oscillation patterns.

1.1.2 Majorana Mass

The direct evidence for neutrino masses from oscillation experiments poses the question of constructing neutrino mass terms in the Lagrangian. In the Standard Model, all fermions acquire their masses via Yukawa coupling to the Higgs doublet through spontaneous symmetry breaking (SSB) [12]. The result is a gauge invariant Dirac mass term that involves both left-handed and right-handed chiral fermion states. Since the weak force only interacts with left-handed states, a right-handed neutrino ν_R is expected to be a gauge singlet that is sterile and does not participate in any Standard Model interactions. While there is no direct evidence of the existence of right-handed neutrinos yet, it is trivial to construct Dirac mass terms for neutrinos in an analogous way to other fermions:

$$\mathcal{L}_D = -m_D(\overline{\nu}_R\nu_L + \overline{\nu}_L\nu_R), \quad (1.3)$$

where $\mathcal{L}_D$ is the mass Lagrangian, m_D is the Dirac mass and ν_L (ν_R) is the left(right)-handed neutrino state. However, if we were to accept that all the neutrino masses are Dirac masses only, then the sheer smallness of neutrino masses would require exceptionally small Yukawa coupling constants in comparison to other leptons. It is, therefore, more natural to look for alternative mass generation mechanisms from a theoretical perspective.

Being gauge singlets, right-handed neutrinos (and left-handed antineutrinos) can have so-called Majorana mass terms in addition to Dirac masses in the Lagrangian, without breaking gauge invariance. The origin of such terms can be explored from a field perspective under the Dirac equation

$$(i\gamma^\mu\partial_\mu - m)\Psi = 0. \quad (1.4)$$

The Dirac γ -matrices are required to satisfy two conditions. First, they need to obey Clifford algebra $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$; second, the implied Hamiltonian from the Dirac equation should be hermitian, meaning that one of the γ -matrices, γ_0 , is hermitian, while the other γ_i matrices are anti-hermitian. It is worth noting that these conditions do not specify the representation of Dirac matrices. If the Dirac matrices are purely imaginary in a particular representation, the Dirac equation reduces to a real equation. Such a representation is referred to as

the Majorana representation, and the fermion field is a Majorana fermion. The Majorana representation of Dirac matrices $\tilde{\gamma}^\mu$ can be written in terms of Pauli matrices σ^i :

$$\begin{aligned}\tilde{\gamma}^0 &= \begin{bmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{bmatrix}, & \tilde{\gamma}^1 &= \begin{bmatrix} i\sigma^1 & 0 \\ 0 & i\sigma^1 \end{bmatrix}, \\ \tilde{\gamma}^2 &= \begin{bmatrix} 0 & \sigma^2 \\ -\sigma^2 & 0 \end{bmatrix}, & \tilde{\gamma}^3 &= \begin{bmatrix} i\sigma^3 & 0 \\ 0 & i\sigma^3 \end{bmatrix}.\end{aligned}\tag{1.5}$$

A general representation of Dirac matrices can be related to the Majorana representation through a similarity transformation using a unitary matrix, and the corresponding fermion field satisfies the following reality condition as imposed by the real Dirac equation:

$$U^\dagger \Psi = (U^\dagger \Psi)^*.\tag{1.6}$$

By defining the charge conjugation matrix with $UU^T \equiv \gamma_0 C$, the Majorana fermion field can be defined to satisfy the Majorana condition:

$$\Psi = \Psi^c \equiv \gamma_0 C \Psi^*,\tag{1.7}$$

where Ψ^c is the “charge conjugate” of Ψ . This means the Majorana fermion is the same as its antifermion, which is also in agreement with the reality condition of the Dirac equation.

The key difference between a Majorana fermion and a Dirac fermion is the allowed mass terms in the Lagrangian. Mass terms are Lorentz scalars, and for charged fermions, they can only be constructed by contracting two spinors with different chirality:

$$\mathcal{L}_D = -m_D \bar{\Psi} \Psi = -m_D (\bar{\Psi}_L \Psi_R + \bar{\Psi}_R \Psi_L),\tag{1.8}$$

where Ψ is a 4-spinor and $\Psi_{L,R} = \frac{1 \mp \gamma_5}{2} \Psi$ denote the left/right handed projections of Ψ with definite chirality. Since neutrinos have no charge, it is possible to contract Ψ with itself without violating charge conservation. To construct a Lorentz scalar mass term, one requires the charge conjugate of Ψ as defined in Eq. 1.7. Since γ_5 anti-commutes with all other Dirac matrices, Ψ^c has opposite chirality to Ψ with the resulting Majorana mass term

$$\mathcal{L}_M = -\frac{m_L}{2} \left((\bar{\Psi}_L)^c \Psi_L + h.c. \right) - \frac{m_R}{2} \left((\bar{\Psi}_R)^c \Psi_R + h.c. \right).\tag{1.9}$$

For neutrino masses, the Dirac and Majorana mass terms in Eq. 1.8 and Eq. 1.9 can be combined into a single Lagrangian by defining generalised neutrino fields

$$n_L \equiv \begin{bmatrix} \nu_L \\ (\nu_R)^c \end{bmatrix}, \quad (1.10)$$

where ν_L and ν_R are the generalised 4-spinors with $N = 3$ flavours:

$$\nu_L \equiv \begin{bmatrix} \nu_{eL} \\ \nu_{\mu L} \\ \nu_{\tau L} \end{bmatrix}, \quad \nu_R \equiv \begin{bmatrix} \nu_{eR} \\ \nu_{\mu R} \\ \nu_{\tau R} \end{bmatrix}. \quad (1.11)$$

The combined Lagrangian under this notation is

$$\mathcal{L}_{D+M} = -\frac{1}{2} \overline{(n_L)^c} \mathcal{M} n_L + h.c., \quad \mathcal{M} = \begin{pmatrix} \mathcal{M}_L & \mathcal{M}_D^T \\ \mathcal{M}_D & \mathcal{M}_R \end{pmatrix}. \quad (1.12)$$

Both the Dirac masses $\mathcal{M}_D$ and Majorana masses $\mathcal{M}_L$ and $\mathcal{M}_R$ are $N \times N$ matrices, with a total of $2N$ non-degenerate spinors. Each of these spinors transforms into itself under CPT, meaning that it is the antiparticle of itself and is therefore a Majorana fermion. One can easily see that the standard Dirac neutrinos are a special case where both $\mathcal{M}_L$ and $\mathcal{M}_R$ are zero.

1.1.3 The Seesaw Mechanism

The seesaw mechanism provides a simple extension of the Standard Model that enables small neutrino masses to arise naturally in the existence of Majorana neutrino mass terms. There exist Type-I, Type-II, and Type-III seesaw mechanisms, forming the tree-level completions of the dimension-5 ‘‘Weinberg operator’’ [13]. The latter two types are not discussed within the context of this work and any future reference to the seesaw mechanism can be considered as Type-I only. The minimal construction of the mechanism postulates the existence of heavy right-handed Majorana neutrino states, and utilises the general mass matrix in Eq. 1.12 with both Dirac and Majorana terms. This can be illustrated for the simple one-generation case by defining the following Majorana fields

$$\xi \equiv \nu_L + \nu_L^c, \quad \eta \equiv \nu_R + \nu_R^c, \quad (1.13)$$

and the general mass matrix becomes

$$\mathcal{L}_{D+M} = -\frac{1}{2} \begin{pmatrix} \bar{\xi} & \bar{\eta} \end{pmatrix} \begin{pmatrix} m_L & m_D \\ m_D & m_R \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}, \quad (1.14)$$

where m_D is the Dirac mass and m_L and m_R are the Majorana masses for the left and right-handed neutrino fields ν_L and ν_R . Provided that $m_D, m_L \ll m_R$, a simple diagonalisation gives the following two mass eigenvalues

$$m_1 = m_L - \frac{m_D^2}{m_R}, \quad m_2 = m_R + \frac{m_D^2}{m_R}. \quad (1.15)$$

The Standard Model left-handed neutrinos transform with left-handed leptons as $SU(2)_L$ gauge doublets, therefore ν_L cannot by itself have Majorana mass (i.e. $m_L = 0$). This is due to the lack of gauge invariance of a purely left-handed Majorana neutrino mass term, simply because the $SU(2)_L$ transformation mixes neutrino and charged-lepton states. This is not the case for a right-handed component of a neutrino field, which is a gauge singlet and can have explicit Majorana mass terms. The existence of such a particle is well motivated in grand unification theories (GUTs) with an $SO(10)$ gauge group, typically having an energy scale on the order of $m_R \approx 10^{15}$ GeV [14]. If we then set the Dirac mass of neutrinos to be similar to quark mass, then the lighter of the two mass eigenvalues becomes

$$m_1 = -\frac{m_D^2}{m_R} \approx 10^{-12} \text{ eV}. \quad (1.16)$$

One can see that increasing the mass of the sterile right-handed neutrino reduces that of the observed neutrino mass eigenvalue, hence the “seesaw” nomenclature. The mass eigenstates can be explicitly written as

$$\nu_1 = \xi \cos \theta - \eta \sin \theta, \quad \nu_2 = \xi \sin \theta + \eta \cos \theta, \quad (1.17)$$

where $\tan \theta = m_D/m_R$. Since both ξ and η are by definition Majorana fields, the mass eigenstates also satisfy the Majorana condition $\nu = \nu^c$ and are Majorana fermions.

1.2 The Majoron

1.2.1 Motivating the Majoron

The introduction of right-handed Majorana neutrinos brings important consequences. While the Majorana mass term $m_R \overline{\nu_R^c} \nu_R$ does not violate any Standard Model gauge symmetry, it explicitly violates the conservation of lepton number, L . In addition, a Majorana neutrino inevitably leads to processes such as neutrinoless double beta decay ($0\nu\beta\beta$), which also violates L -conservation by two units. From a theoretical perspective, L -violation by itself is not a major problem. The global $U(1)_L$ symmetry associated with lepton number conservation is not pre-imposed in the Standard Model. It is an accidental symmetry that arises in the Standard Model Lagrangian when only considering low-order operators, and is broken by anomalies at the quantum level. There is no reason to expect physics beyond the Standard Model to respect L -conservation. However, processes related to the Majorana neutrino, such as $0\nu\beta\beta$, also violate $B - L$ (the difference between baryon number B and lepton number L) conservation. While still being an accidental symmetry in the Standard Model, the $U(1)_{B-L}$ symmetry associated with $B - L$ conservation is a much more robust symmetry than $U(1)_L$ or $U(1)_B$ individually. The anomalies that would break B -conservation and L -conservation always cancel each other, leaving the $B - L$ conserved. In fact, it is the only anomaly-free global symmetry in the Standard Model and has the potential to be promoted to a gauge symmetry [15]. Therefore, there is strong theoretical motivation to expect a viable extension of the Standard Model to have a Lagrangian that respects the $U(1)_{B-L}$ symmetry.

For $B - L$ violating processes to be possible while keeping the $U(1)_{B-L}$ symmetry in the Lagrangian, perhaps the most natural approach is to consider global spontaneous symmetry breaking (SSB). In other words, while the Lagrangian respects the $U(1)_{B-L}$ global symmetry, the state does not. The Goldstone theorem states that for each broken generator of the symmetry group, there is a corresponding massless Goldstone boson. In the case where $U(1)_{B-L}$ is broken, the resulting Goldstone boson is commonly referred to as the Majoron.

The Majoron is a very compelling extension of the Standard Model. It requires very little

new physics, yet it offers potential solutions to the following important physics problems:

- **Leptogenesis** – A broken $U(1)_{B-L}$ leads to L -violating decays of heavy Majorana neutrinos via Majoron in the early universe. Such decays generally happen at or above the Seesaw scale with $M_R \sim 10^{12}$ GeV. This introduces some level of lepton asymmetry in the early universe, which can be subsequently converted to baryon asymmetry via the sphaleron process (a high-order $B - L$ conserving process) in the Standard Model [16]. As the universe expands, these baryons exit thermal equilibrium with other particles and continue to decay or annihilate. However, this freeze-out mechanism still leaves a relic baryon density that could potentially explain the baryon asymmetry in the universe [17].
- **Neutrino Mass Generation** – As mentioned above, an explicit Majorana mass term violates L -conservation (and in turn violates $B - L$ conservation). With the introduction of the global SSB mechanism and the associated Majoron, the theory's Lagrangian can respect the $U(1)_{B-L}$ symmetry while still allowing Majorana mass terms to arise from SSB. It is also worth noting that in GUTs with an $SO(10)$ symmetry group, Majorana neutrino and the Seesaw mechanism arise naturally, and the $U(1)_{B-L}$ is broken spontaneously [14].
- **Dark Matter** – While the Majoron is naturally massless, it is possible to generate mass for it to become a potential dark matter candidate. If $U(1)_{B-L}$ is after all an approximate symmetry with very small explicit breaking terms (or anomaly terms), the Majoron then becomes a pseudo-Goldstone boson with mass [18]. If this is the case, it is possible to have Majorons with the correct relic density of dark matter via the freeze-in mechanism. This is analogous to the more famous dark matter candidate the axion, which is a pseudo-Goldstone boson from SSB of the global $U(1)_{PQ}$ Peccei-Quinn symmetry.

The experimental endeavor to search for Majoron-emitting processes has been ongoing for decades. The main process that has been looked for is the Majoron-emitting double beta decay, which this work will focus on. For completeness of the context, in recent years some

experiments that primarily look for $\mu \rightarrow e$ conversion have also proposed the possibility to look for the $\mu \rightarrow e\phi$ channel, where ϕ is the emitted Majoron [19].

1.2.2 Double Beta Decay

An unstable nucleus may undergo two simultaneous β -decay, emitting two electrons and two anti-neutrinos at once

$$(A, Z) \rightarrow (A, Z + 2) + 2e^- + 2\bar{\nu}_e, \quad (1.18)$$

where A is the atomic number, and Z is the proton number.

Being a second-order weak interaction, the process is heavily suppressed with one of the longest known half-lives for nuclear decay, typically in the range of $10^{19} - 10^{21}$ yr. Furthermore, this process can only take place in certain natural isotopes, whereby the first order β -decay is forbidden. Since the pairing term in the nuclear binding energy E_b is positive for atoms with odd A and Z , it is possible for the $Z - 1$ daughter isobar to have a higher binding energy than its parent, while the $Z - 2$ isobar has a lower one. Therefore, the first order β -decay cannot occur due to energy conservation but the double beta decay ($2\nu\beta\beta$) is allowed. This process is only possible for isotopes with A and Z that are both even. The energy released in the process is denoted as the Q-value, $Q_{\beta\beta}$, which is simply the difference in the nuclear binding energy of the parent and daughter nuclei:

$$Q_{\beta\beta} = E_b(A, Z) - E_b(A, Z + 2). \quad (1.19)$$

With the possibility of neutrinos being Majorana fermions, an alternative process was soon suggested, known as the neutrinoless double beta decay ($0\nu\beta\beta$) [20]. The simplest mechanism by which $0\nu\beta\beta$ can happen is via the light neutrino exchange, where the decay is mediated by a virtual Majorana neutrino propagator as illustrated by the Feynman diagram Figure 1.1. A Majorana neutrino is required in this case due to the chiral nature of the weak interaction, allowing only a left-handed neutrino and a right-handed antineutrino to connect to outgoing electrons.

There is a direct correspondence between $0\nu\beta\beta$ and the Majorana neutrino mass regardless of the underlying mechanism, as established by the “Black Box” theorem. It is simple to prove

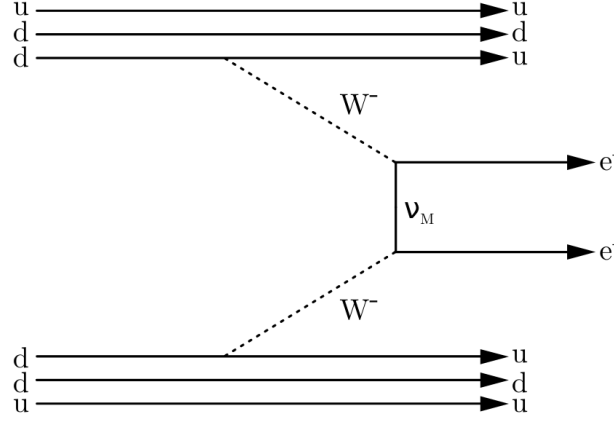


Figure 1.1: Feynman diagram of a $0\nu\beta\beta$ process mediated by the exchange of a light Majorana neutrino, here denoted by ν_M .

the theorem for the one-generation case. For the forward direction of the correspondence, one can consider the following virtual vacuum process that produces quarks and electrons:

$$0 \rightarrow uud\bar{d}\bar{e}^-e^- . \quad (1.20)$$

By crossing symmetry, a non-zero amplitude of $0\nu\beta\beta$ also leads a non-zero amplitude of the above vacuum process. Assuming that any extension of the Standard Model should include the known interaction between the W boson, u and d quarks, electron and neutrino, one can construct a high-order correction to the neutrino propagator as shown in Figure 1.2. The two external legs being ν_e and $\bar{\nu}_e$ respectively shows that such a correction gives rise to a Majorana mass component to the neutrino, proving the forward direction of the correspondence.

Conversely, one can look at the light neutrino exchange mechanism in Figure 1.1 and show that a Majorana mass component inevitably leads to a non-zero amplitude of $0\nu\beta\beta$. The theorem can also be generalised to N-flavours to show a one-to-one correspondence between entries of the Majorana mass matrix and the amplitude matrix of $0\nu\beta\beta$ of different flavours [21]. Therefore, observation of $0\nu\beta\beta$ in any isotope will be a direct piece of evidence of the Majorana neutrinos.

A family of alternative double beta decays has been built upon the idea of global SSB of

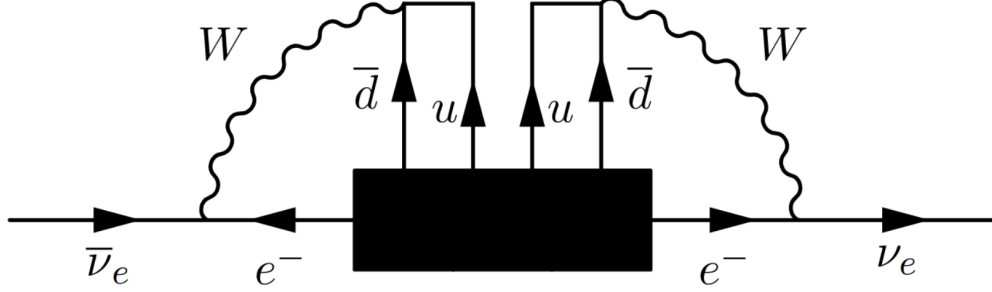


Figure 1.2: Illustration of Black Box theorem for the one-generation case. The diagram represents the contribution of a general underlying physical process encompassed by the “black box” operator to the Majorana mass of a neutrino propagator. Figure from Ref. [22].

$U(1)_{B-L}$ and the emission of a Majoron. The general decay process is as below:

$$(A, Z) \rightarrow (A, Z + 2) + 2e^- + \phi (+ \phi). \quad (1.21)$$

The last bracket above indicates the possibility of emitting a second Majoron, which will be discussed later. One should note that while Majoron-emitting double beta decay ($0\nu\beta\beta\phi$ or $0\nu\beta\beta\phi\phi$) does not emit any neutrino, it is inherently different from $0\nu\beta\beta$. Therefore, the observation of one does not necessarily imply the other, and the link between the two is model-dependent.

1.3 Majoron Models

1.3.1 Standard Singlet Majoron Model

The first model that explored the possibility of Majoron emission was proposed by Chikashige, Mohapatra, and Peccei in 1981 [23]. The model postulates the existence of two separate complex scalar fields, the Standard Model Higgs doublet Φ and a new singlet field χ . For this reason, the model is commonly referred to as the singlet Majoron model. The model further assumes the same structure of neutrino masses and states as the Seesaw mechanism in Section 1.1.3. In a simple one-generation case, the Yukawa coupling terms under the two

separate scalar fields are:

$$\begin{aligned}\mathcal{L}_1 &= -h_1(\bar{\psi}_L\Phi\nu_R + \bar{\nu}_R\Phi^\dagger\psi_L), \\ \mathcal{L}_2 &= -h_2(\chi\bar{\nu}_R^c\nu_R + \chi^\dagger\bar{\nu}_R\nu_R^c).\end{aligned}\tag{1.22}$$

Assuming that the Lagrangians respect the global $U(1)_{B-L}$ symmetry, the expression of $\mathcal{L}_2$ means that χ carries a lepton number of 2. One may rewrite χ as

$$\chi = \frac{1}{\sqrt{2}}(\langle\chi\rangle + \rho + i\phi),\tag{1.23}$$

where $\langle\chi\rangle$ is the vacuum expectation value (VEV) of χ while ρ and ϕ are massive scalar and massless Goldstone scalar respectively, the last of which is the Majoron field. If $\langle\chi\rangle$ is non-zero, $\mathcal{L}_2$ simply becomes the Majorana mass terms of the general mass Lagrangian, with $m_R = \frac{1}{\sqrt{2}}h_2\langle\chi\rangle$. The Majoron field couples to the light ξ and the heavy η Majorana neutrino fields as

$$\mathcal{L}_{\phi\nu} = \frac{1}{\sqrt{2}}ih_2\phi\left[\bar{\eta}\gamma_5\eta - \left(\frac{m_D}{m_R}\right)(\bar{\eta}\gamma_5\xi + \bar{\xi}\gamma_5\eta) + \left(\frac{m_D}{m_R}\right)^2\bar{\xi}\gamma_5\xi\right].\tag{1.24}$$

The important message here is that the Majoron only couples strongly to the heavy Majorana neutrino state η and any coupling to the lighter η state is suppressed by the seesaw scale m_R .

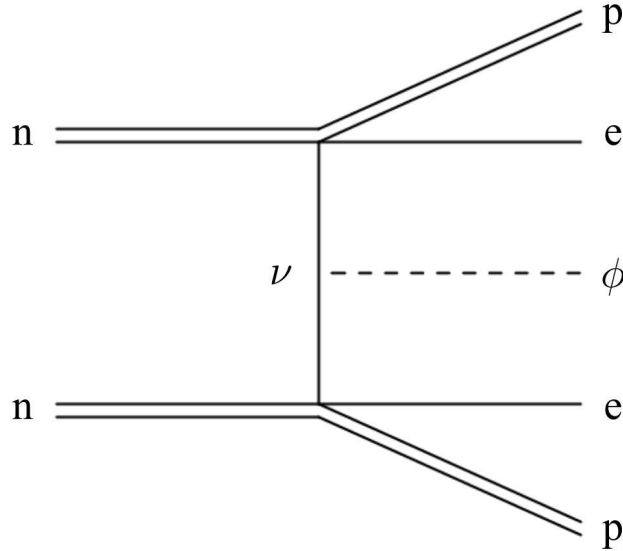


Figure 1.3: Diagram of neutrinoless double beta decay with a single Majoron emission.

The singlet model is, to a large extent, the standard mechanism when considering Majoron emission. For the completion of the context, there were also some classical Majoron models being proposed at around the same time as the singlet model. An example of such is the triplet model proposed by Gelmini and Roncadelli [24]. It postulates a complex triplet scalar field in addition to the Standard Model Higgs doublet, without the need to introduce right-handed Majorana neutrinos. However, these models are generally disfavoured by LEP’s invisible Z width measurement [25]. A Majoron from the triplet model is expected to contribute to an equivalence of two extra light neutrino species, while LEP’s measurement is in strong agreement with only three light-neutrino species as in the Standard Model [26].

1.3.2 Double and Charged Majorons

It is possible for a model’s field content to result in the emission of two Majorons simultaneously. One way to achieve this is by introducing a single scalar field χ and three extra left-handed neutrinos, $N_{\pm}$ and N_0 , that transform as singlets under the $SU(2) \times U(1)$ electroweak transformation. In this formalism, double Majoron emission can occur via the exchange of the sterile neutrino between Standard Model neutrinos, as can be seen in the Feynman diagram in Figure 1.4. A comprehensive overview of ways to achieve double Majoron emission, including those involving supersymmetry (SUSY) can be found in [27].

In more recent years, due to the exceedingly stringent limits on the half-life of $0\nu\beta\beta$, the VEV of new scalars in many potential Majoron models are severely constrained and are subject to the naturalness problem when comparing with the Standard Model Higgs VEV. To circumvent this problem, a new class of charged Majoron models has been proposed in which the Majoron carries the lepton number itself. Such models typically require more complex field structures and let SSB take place at a higher level, resulting in the global $U(1)_{B-L}$ as a residual symmetry. For example, one can expand the Standard Model gauge group by a global $SU(2) \times U(1)$ then SSB to $U(1)_{B-L}$, in an analogous way to how the $SU(2) \times U(1)$ electroweak symmetry is broken to $U(1)_{EM}$. The significance here is that $U(1)_{B-L}$ remains as a symmetry that no longer goes through SSB, and the emitted bosons in these models are no longer Goldstone bosons [28]. For the rest of this work, the word

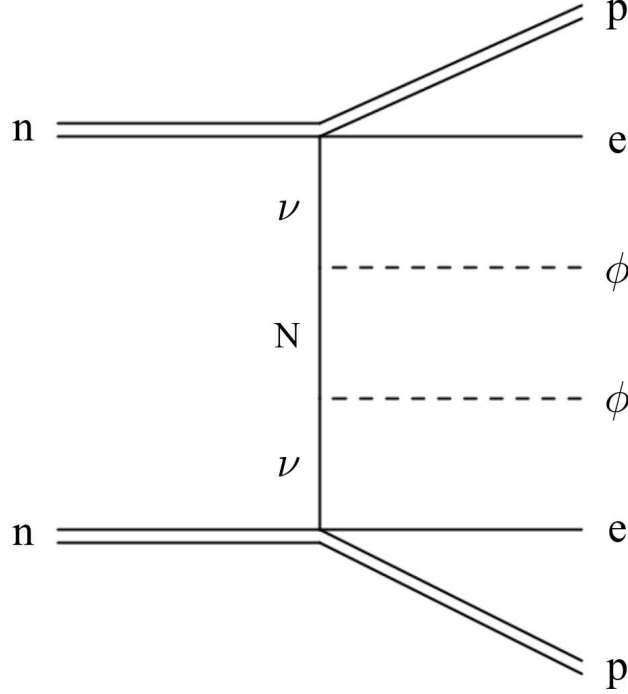


Figure 1.4: Diagram of a possible arrangement of double-Majoron mode. The decay process is mediated by additional left-handed sterile neutrino species to the Standard Model.

“Majoron” generally refers to any Majoron-like boson that shares a similar experimental signature as the standard singlet Majoron. Models with charged Majorons are subject to less fine-tuning of the VEV of new scalar fields, at the cost of completely forbidding the $B - L$ violating $0\nu\beta\beta$.

1.3.3 Classification of Majoron Models

There is a plethora of theoretical models that postulate processes with Majoron emission, yet with very different underlying mechanisms. This brings the imminent need to classify Majoron models in an organised fashion. The community mostly uses the same formalism as in [27] and classifies the models by asking a few key questions regarding the nature of the Majoron. These questions include the following:

- Is the $U(1)_{B-L}$ symmetry broken in the model?
- Does the model permit the standard $0\nu\beta\beta$?

- What is the lepton number of a Majoron in the model?
- How many Majorons are emitted in the decay process?
- Is the Majoron a Goldstone boson?

Those models with SSB of $U(1)_{B-L}$ permitting $0\nu\beta\beta$ are denoted as Class I. The others that have a charged Majoron that preserves $U(1)_{B-L}$ and forbids $0\nu\beta\beta$ are denoted as Class II models. A summary of this classification is illustrated in Table 1.1. The final column of the table shows the spectral index associated with each class of the Majoron model, which will be discussed in more detail.

Table 1.1: Classification of Majoron models. The notations follow those in Ref. [27].

Model	L_e symmetry	$0\nu\beta\beta$	L	Decay Mode	Goldstone boson	Spectral Index
IA	Broken	Yes	N.A.	N.A.	N.A.	N.A.
IB	Broken	Yes	0	ϕ	No	1
IC	Broken	Yes	0	ϕ	Yes	1
ID	Broken	Yes	0	$\phi\phi$	No	3
IE	Broken	Yes	0	$\phi\phi$	Yes	3
IF	Broken	Yes	0	ϕ	bulk field	2
IIA	Unbroken	No	N.A.	N.A.	N.A.	N.A.
IIB	Unbroken	No	-2	ϕ	No	1
IIC	Unbroken	No	-2	ϕ	Yes	3
IID	Unbroken	No	-1	$\phi\phi$	No	3
IIE	Unbroken	No	-1	$\phi\phi$	Yes	7
IIF	Unbroken	No	-2	ϕ	gauge boson	3

1.3.4 Spectral Index

The heavily suppressed coupling between Majoron and Standard Model particles means that they generally escape the detector medium without interaction. If we consider energy as the

observable, the sum of kinetic energies of the two emitted electrons is expected to follow a continuous energy spectrum. The predicted energy spectrum is model-dependent and as it turns out, the spectral shape can be characterised by a single integer, which is referred to as the spectral index. One can arrive at this conclusion by considering the differential decay rate of a general double beta decay process:

$$d\Gamma(\beta\beta) = \frac{(G_F \cos \theta_C)^4}{4\pi^3} |\mathcal{A}(\beta\beta)|^2 d\Omega(\beta\beta), \quad (1.25)$$

where G_F is the Fermi constant and θ_C is the Cabbibo angle. $\mathcal{A}(\beta\beta)$ and $d\Omega(\beta\beta)$ is the nuclear matrix element and the differential phase space respectively, both of which are specific to the double beta decay process. This factorisation separates all the energy dependence of the decay rate into $d\Omega(\beta\beta)$. For any Majoron-emitting double beta decay, the differential phase space takes the form

$$d\Omega(\beta\beta) = \frac{1}{64\pi^2} (Q_{\beta\beta} - \epsilon_1 - \epsilon_2)^n [p_1 \epsilon_1 F(\epsilon_1) d\epsilon_1] [p_2 \epsilon_2 F(\epsilon_2) d\epsilon_2], \quad (1.26)$$

where ϵ_1 , ϵ_2 , p_1 and p_2 are the energy and magnitude of three-momentum of the two outgoing electrons, and $F(\epsilon)$ is the normalised Fermi function. This expression assumes that the Majoron in the model is massless. If massive, the $(Q_{\beta\beta} - \epsilon_1 - \epsilon_2)$ part of the expression should be replaced by $((Q_{\beta\beta} - \epsilon_1 - \epsilon_2)^2 - m^2)^{1/2}$.

It is evident from Eq. 1.26 that the differential decay rate follows a power law with an integer spectral index, n . Majoron-emitting models typically have $n = 1, 2, 3, 7$, and this is the standard set of spectral indices that a double beta decay experiment will search for. If an excess in the energy spectrum with a particular value of n is observed, it will provide essential information on shortlisting the favoured Majoron model. For example, models with single Majoron emissions always have $n = 1, 2, 3$, while double Majoron emissions are always associated with $n = 3, 7$ [27]. Since most Majoron models have incompatible field contents with each other, those models with different spectral indices to the observed one will be strongly disfavoured. However, taking energy as the observable means that one cannot distinguish between models with the same n , leaving still a set of models that are all compatible with the observation. Also, the spectral index does not provide information on whether the

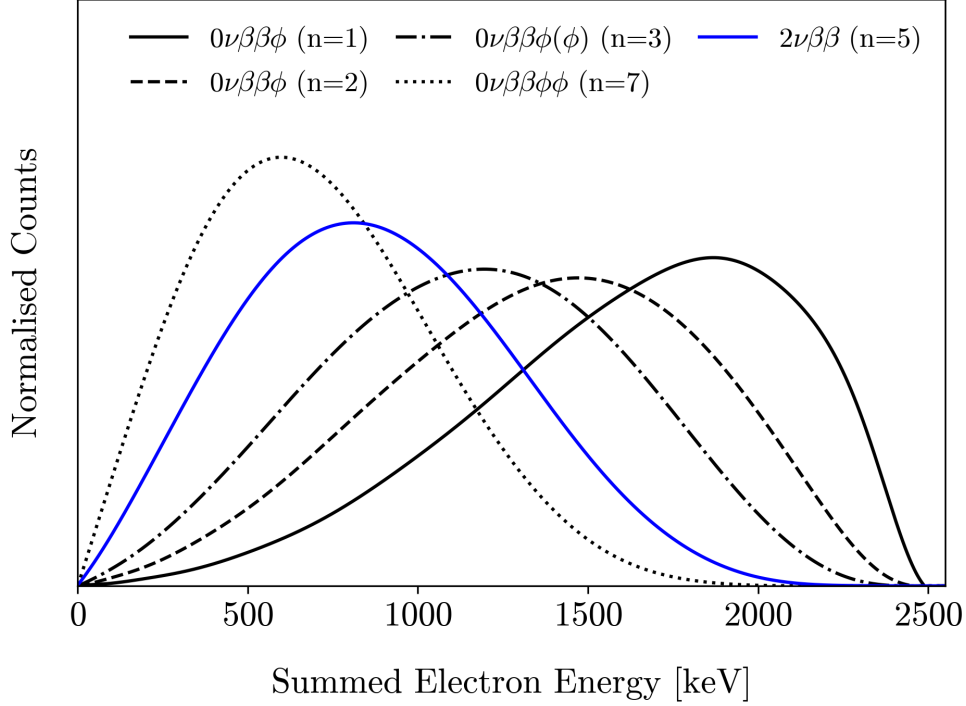


Figure 1.5: Energy spectra for different double beta decay modes in ^{136}Xe , characterised by their spectral indices. The detectable energy of a double beta decay event is the sum of kinetic energies of the two emitted electrons, and is considered as the observable that differentiates different decay modes. Each energy spectrum is normalised to unit area, and the $Q_{\beta\beta}$ value of the isotope under consideration marks the end-point of the energy spectra.

Majoron model is of Class I or Class II. Such a distinction will require information on the nature of neutrino mass from $0\nu\beta\beta$ searches.

Figure 1.5 shows the shape of the visible energy spectra of Majoron-emitting decays, together with the Standard Model $2\nu\beta\beta$ that has an equivalent spectral index of $n = 5$. The $\beta\beta$ isotope under consideration in the figure is ^{136}Xe , with a $Q_{\beta\beta}$ value of 2458 keV [29], which marks the end-point of the energy spectra. With a larger spectral index, the spectrum peaks at lower energy due to the extra degrees of freedom available in the phase space of end products. Since a nucleus that can decay via $0\nu\beta\beta\phi$ also decays via $2\nu\beta\beta$, it is both the signal source and a major background. It is therefore expected that an experimental search

based on the energy observable is more sensitive to a lower spectral index, as the signal energy spectrum is more distinct from the $2\nu\beta\beta$ background.

1.4 Majoron-Neutrino Coupling Constant

The experimental signature of $0\nu\beta\beta\phi$ consists of two electrons with a summed energy continuum. The energy spectrum follows an integer spectral index. In the simple picture with no background events, the number of observed signal events N_s can be translated to a corresponding half-life $T_{1/2}$ via:

$$T_{1/2} = \frac{\epsilon N_{\beta\beta} T}{N_s} \ln 2, \quad (1.27)$$

where ϵ is the signal detection efficiency, $N_{\beta\beta}$ is the number of $\beta\beta$ isotope atoms under observation and T is the total measurement time.

This picture is not realistic in practice, as a search for $\mathcal{O}(\text{MeV})$ electron recoils will inevitably have background events in any detector technology. With N events measured in total, N_b of them could be background events and the remaining N_s could be signal events. One would require sufficient statistical significance in the observed N_s to claim the discovery of $0\nu\beta\beta\phi$ and measure its half-life. On the other hand, if the estimated value of N_s value is not statistically significant to claim discovery, it may still exclude half-lives to a certain lower limit. This ability to exclude a hypothesised half-life is referred to as the sensitivity of an experiment. The standard in the field is to report the sensitivity at 90% confidence level (CL).

Half-life limits from different experiments are not directly comparable due to the difference in nuclear physics and phase space products of $0\nu\beta\beta\phi$ from different $\beta\beta$ isotopes. In order to obtain a performance metric that is generally applicable to different experimental techniques, the half-life of a $0\nu\beta\beta\phi$ process can be expressed as

$$[T_{1/2}]^{-1} = g_A^4 G_{m,n} |\langle g_\phi \rangle|^{2m} |M_{m,n}|^2, \quad (1.28)$$

where g_A is the axial vector coupling constant, $G_{m,n}$ is the phase space factor (PSF) that takes into account all integrals of the phase space, $M_{m,n}$ is the nuclear matrix element (NME)

that accounts for the nuclear physics of the entire process, and g_ϕ is the Majoron-neutrino coupling constant. Detailed studies have been performed for theoretical calculation of $G_{m,n}$ and $M_{m,n}$, both of which are dependent on the number m of Majorons emitted and the spectral index n [30, 31]. Due to the different (“bulk field”) origin of the $n = 2$ mode, derivations of expressions of NME and PSF are not provided in literature. There are also large theoretical uncertainties coming from the value of g_A due to the unconfirmed level of quenching (reduction from the free space value) [8]. Nevertheless, provided the same set of parameter values are selected, the Majoron-neutrino coupling constant g_ϕ can be directly compared between different isotopes. Table 1.2 lists the current best limits on the upper bound of the Majoron-neutrino coupling constant for ^{76}Ge , ^{82}Se , ^{100}Mo , ^{130}Te and ^{136}Xe , as obtained by various experiments including GERDA, CUPID, NEMO, CUORE and EXO. These isotopes are among the most widely studied by different experiments and provide more competitive limits compared to other $\beta\beta$ isotopes. The limits for $n = 1$ and $n = 3$ single-Majoron modes are significantly more stringent as a consequence of the $\mathcal{O}(10^3)$ larger NME values in comparison to double-Majoron modes [32]. Currently, ^{136}Xe provides the most competitive results for all commonly searched Majoron-emitting modes.

Table 1.2: Upper bound of Majoron-neutrino coupling constant, calculated from lower limits on half-lives of ^{76}Ge [33], ^{82}Se [34], ^{100}Mo [35], ^{130}Te [36, 37] and ^{136}Xe [38] at 90% CL. The PSF and NME values are taken from Ref. [30] and Ref. [31], respectively. The calculation assumes a quenched scheme where $g_A = 1$.

Isotope	n=1	n=3 (ϕ)	n=3 (2ϕ)	n=7
^{76}Ge	3.5×10^{-5}	3.4×10^{-2}	1.7	1.9
^{82}Se	2.8×10^{-5}	2.5×10^{-2}	1.5	1.4
^{100}Mo	4.7×10^{-5}	2.4×10^{-2}	1.5	3.0
^{130}Te	8.8×10^{-5}	8.7×10^{-2}	3.8	2.6
^{136}Xe	0.6×10^{-6}	0.6×10^{-2}	0.8	1.1

1.5 Detection Technologies

The remainder of this chapter discusses the main technologies used in the current and next-generation searches for double beta decays. While the primary focus of many double beta experiments is to observe the standard $0\nu\beta\beta$ decay mode, the same detector technology is usually versatile enough to be used to search for other double beta decay processes including $0\nu\beta\beta\phi$. Due to the requirements on the physical and chemical properties of the detector medium, each detection technology is typically very specific to the $\beta\beta$ isotope under consideration.

1.5.1 Bolometers

A thermal bolometer, or cryogenic calorimeter, utilises the tiny temperature rise from a particle interaction within a crystal lattice. The crystal is operated at an ultra-cryogenic temperature, roughly on the order of mK, and coupled directly to a temperature sensor. The low base temperature allows the detector to be sensitive to temperature changes of $\mathcal{O}(0.1 \text{ mK})$. For double beta decay searches, crystals of compounds that contain $\beta\beta$ isotopes such as ^{82}Se , ^{100}Mo and ^{130}Te are grown with low radioactive contamination. A variant of this detector technology is the scintillating bolometer, whereby the detector medium produces both a light and a heat signal. Examples of such a detector medium include some scintillating crystals based on Se, Mo and Cd compounds. The light signal can be detected using an auxiliary optical bolometer, which is then analysed together with the heat signal for particle identification and background rejection [39].

An example of a pure thermal bolometer experiment for double beta decay is the Cryogenic Underground Observatory for Rare Events (CUORE) [40]. The experiment operates at Laboratori Nazionali del Gran Sasso (LNGS) and utilises TeO_2 crystals to investigate the decays of ^{130}Te . The experiment is now in the process of transitioning to CUORE Upgrade with Particle IDentification (CUPID), a future tonne-scale scintillator bolometric experiment [41]. The first demonstrator of the project, CUPID-0, has published the current best limit on Majoron-emitting double beta decays of ^{82}Se [34]. The corresponding upper bounds

on g_ϕ are calculated and listed in Table. 1.2. This result is based on just 9.95 kg·yr exposure, demonstrating the potential of scintillating bolometers in this field.

1.5.2 Tracking Calorimeters

A tracking calorimeter, as the name suggests, is capable of tracking the electron paths of double beta decay, as well as measuring the total decay energy. A notable previous experiment of this type is the Neutrino Ettore Majorana Observatory (NEMO), located at the Laboratoire Souterrain de Modane (LSM). NEMO used thin foils of $\beta\beta$ isotope as the source material and placed them between gaseous layers to achieve tracking, followed by a surrounding calorimeter layer for energy measurement. Its ability to track electron paths rejects background events with distinct vertices. This also allows it to measure the angular distribution of the emitted electrons, providing an additional observable to the traditional energy-only analysis for $0\nu\beta\beta\phi$.

One major advantage of the NEMO experiment is the versatility of changing the $\beta\beta$ source, thanks to its separation of source material from the detection medium. The experiment has produced $0\nu\beta\beta\phi$ half-life limits for ^{82}Se , ^{96}Zr , ^{100}Mo , ^{116}Cd and ^{130}Te [35, 42, 43]. Amongst these results, the ^{100}Mo and ^{130}Te limits on g_ϕ are relatively competitive, as shown in Table 1.2. Its successor, SuperNEMO, has already completed the construction of its demonstrator module and is planned to feature reduced background rates with a larger design. One restriction of this approach is that the $\beta\beta$ isotope of interest has to be formed into thin foils. This excludes some of the most competitive isotopes in $0\nu\beta\beta\phi(\phi)$ searches such as ^{76}Ge or ^{136}Xe in Table 1.2. The scalability of ^{76}Ge - and ^{136}Xe -based experiments are expected to be the main driving force to push for more competitive upper bounds on g_ϕ . Nevertheless, the versatility of searching for $0\nu\beta\beta\phi$ with multiple $\beta\beta$ sources remains a major advantage of this detector technology.

1.5.3 Semiconductor Detectors

A semiconductor detector operates on the premise that ionising radiation passing through a semiconductor produces electrons and holes. These charge carriers subsequently drift to the electrodes under an external field, where they are measured as a current signal. In the field of double beta decay searches, High Purity Germanium (HPGe) detectors are one of the leading technologies due to their unrivalled energy resolution of $\sim 0.1\%$ at $Q_{\beta\beta}$ of ^{76}Ge .

Notable experiments of this type include the Germanium Detector Array (GERDA) at LNGS, and the Majorana Demonstrator (MJD) at the Sanford Underground Research Facility (SURF). Based on data collected during Phase I of the experiment, GERDA has placed lower limits on half-lives of $0\nu\beta\beta\phi$ on the order of 10^{23} yr [33]. The ~ 40 kg active mass in GERDA already places ^{76}Ge at a competitive level for setting upper bounds on g_ϕ , with more results expected for the near future after the completion of Phase II data taking [44].

The semiconductor detector technology is also expected to be active in the search for $0\nu\beta\beta\phi$ in the foreseeable future. GERDA and MAJORANA have formed a joint future successor, the Large Enriched Germanium Experiment for Neutrinoless $\beta\beta$ Decay (LEGEND). The first stage of this successor, LEGEND-200, is currently reutilising the GERDA facilities and taking data with 140 kg of germanium detectors. The final stage of the experiment, LEGEND-1000, is designed to comprise five LEGEND-200 modules and is preparing to deploy either at LNGS or SNOLAB.

1.5.4 Scintillator Detectors

Notable experiments that operate on the premise of detecting light produced by particle interactions in liquid scintillator include KamLAND-Zen and the future SNO+ experiment. The former is located in the Kamioka mine and the latter is at SNOLAB. The design of KamLAND-Zen has a central balloon suspended inside a spherical tank, surrounded by water shielding. Organic liquid scintillator loaded with 380 kg of enriched xenon (90% in ^{136}Xe) is used to fill the central balloon. In turn, the SNO+ experiment is planned to use an organic

liquid scintillator doped with 1,300 kg of ^{130}Te [45]. In 2012, KamLAND-Zen set stringent limits on half-lives of $0\nu\beta\beta\phi$ based on 89.5 kg·yr exposure of ^{136}Xe during Phase I of the experiment [46]. The reported $n = 1$ half-life limit of 2.6×10^{24} yr has been world-leading in the field of $0\nu\beta\beta\phi$ searches with ^{136}Xe and was only recently surpassed in 2021 by EXO [38].

An advantage of scintillator detectors is the possibility of operating at scale. As an example, KamLAND-Zen has already been upgraded to its new phase, KamLAND-Zen 800, with a new central balloon, now containing 745 kg of ^{136}Xe [47]. However, a drawback of this detector technology is the limited photon detection efficiency, leading to relatively poor energy resolution ($\sim 5\%$ at $Q_{\beta\beta}$) and a high energy threshold (~ 500 keV). This poses challenges to energy-based background rejection, as well as loss of signal efficiency at the lower end of the energy spectrum.

1.5.5 Time Projection Chambers

A time projection chamber (TPC) measures both the photons emitted by particles from interactions in the detector medium as well as the liberated charge carriers that drift towards an electrode in an electric field (delayed ionisation response). The detector medium is usually a noble element in either gas or liquid state. The detector is capable of both energy and three-dimensional position measurements. This can be achieved by using the hit pattern of photons to reconstruct the interaction position on the horizontal plane, while using the time separation between the light and charge signals to infer the distance traveled by the charge carriers. The position reconstruction technique also allows for distinguishing between single-site and multi-site events, providing a strong rejection tool for events such as background γ interactions.

A commonly used detection medium in a TPC experiment is xenon. Natural xenon contains about 8.9% of ^{136}Xe , 10.4% of ^{134}Xe and 0.1% of ^{124}Xe , all of which are considered viable $\beta\beta$ isotopes. Of these, ^{136}Xe is the most widely used in double beta decay searches due to its relatively high $Q_{\beta\beta}$ and abundance. Dedicated double beta decay experiments such as the Enriched Xenon Observatory (EXO) [48] and its next-generation successor nEXO [49] use

xenon that is enriched to $\sim 90\%$ in ^{136}Xe to optimise their searches. The former was located at the Waste Isolation Pilot Plant (WIPP), and the latter is planned for SNOLAB. EXO has employed a single-phase liquid xenon (LXe) TPC design, with two nearly symmetric drift regions separated by a central cathode grid. At the end of each drift region, there was an array of avalanche photodiodes to collect the scintillation light, while the ionisation was drifted and detected at the crossed wire planes just in front of the photodiodes. On the other hand, nEXO will have a single drift region in the single-phase LXe TPC. It will be using silicon photomultiplier (SiPM) and crossed metal strips for scintillation and ionisation detection respectively. With a complete dataset equivalent to $234.1 \text{ kg}\cdot\text{yr}$ of ^{136}Xe exposure, EXO reported a lower limit of $T_{1/2} > 4.3 \times 10^{24} \text{ yr}$ for the $n = 1$ mode of $0\nu\beta\beta\phi$. It also holds the current best limit for all other commonly searched modes of $0\nu\beta\beta\phi$ in ^{136}Xe [38].

An alternative approach to the LXe-TPC is the high-pressure gaseous xenon TPC (HPXe-TPC). It is more difficult to scale high-density gaseous xenon. However, the HPXe-TPC provides the benefit of an improved energy resolution, as well as the capability of identifying particle track topologies for background rejection [50]. Notable experiments that take this approach include NEXT [51] and PandaX-III [52], both are intended to operate at $\mathcal{O}(100 \text{ kg})$ of enriched xenon.

Another variant of the detector technology is to operate a xenon TPC with both liquid and gaseous phase, or a dual-phase TPC. In this case the ionisation is converted into secondary scintillation (electroluminescence) in a thin layer of gas above the liquid, which is detected with the same photosensors used to detect the primary scintillation. This approach has been adopted in the field of dark matter (DM) direct detection, and has demonstrated strong performance in placing the most stringent limits on DM-nucleon scattering cross sections. Current generation experiments such as LZ [53], XENONnT [54], and PandaX-4T [55] operate with an active xenon mass of multi-tonnes. Potential next generation experiments such as the XLZD Consortium [56] and PandaX-xT [57] are proposed to scale up the active xenon mass by another order of magnitude [58]. While the scalability requirements for DM direct detection means the detection medium is usually xenon at natural abundance, the

sheer scale of the target entails a ^{136}Xe mass that is comparable to that of the dedicated double beta decay experiments. This allows experiments operating on dual-phase TPC detector technology to search for double beta decays, in addition to their main science target of DM detection. This multi-purpose nature is unique to the detector technology, and allows a very broad science case to be investigated with the same investment. This thesis focuses on ^{136}Xe $0\nu\beta\beta\phi$ searches in the LUX-ZEPLIN (LZ) dual-phase xenon TPC experiment. To the author's best knowledge, this thesis provides the first comprehensive $0\nu\beta\beta\phi$ searches in the context of a DM direct detection experiment, providing a solid piece of evidence for the multi-purpose nature of the detector technology.

Chapter 2

The LUX-ZEPLIN Experiment and Liquid Xenon Physics

This chapter focuses on setting the foundation to search for Majoron-emitting double beta decays with the LUX-ZEPLIN (LZ) experiment. As such, the chapter begins with an overview of dual-phase xenon TPCs, the detector technology that LZ utilises. This is followed by a discussion of the key physical processes that take place when particles interact in liquid xenon (LXe). The chapter concludes with details of the LZ experiment that are necessary for presenting the data analysis work in later chapters.

2.1 Dual-phase Time Projection Chambers

A dual-phase time projection chamber (TPC) is a detector technology that uses noble gases in both their liquid and gas phases to detect particle interactions [59, 60]. This detector technology has the ability to measure energy depositions with a high spatial and energy resolution and reconstruct events with their three-dimensional position information. The noble gas of choice is typically argon or xenon, with the latter often used in dark matter and double beta decay searches. Experiments that utilise xenon in a dual-phase TPC have consistently set world-leading results in searches for direct detection of weakly interacting massive particles (WIMPs) [53–55].

A dual-phase xenon TPC generally consists of two distinct regions: a bulk volume filled with liquid xenon (LXe) and a thin layer of gaseous xenon (GXe) at the top of the TPC, typically with height of $\mathcal{O}(\text{mm})$. Particle interactions with the LXe bulk, or “target”, deposits energy in the form of excitation, ionisation and heat. While energy loss to heat cannot be directly measured in a TPC, both excitation and ionisation produce usable signals for analysis. The initial excitation leads to emission of vacuum ultraviolet (VUV) scintillation light, which is promptly detected by photo-detectors. Meanwhile, ionised electrons released by the initial particle interaction can undergo two possible routes: recombination or escape. The electrons that recombine with xenon ions near the primary track lead to additional VUV scintillation. The promptly detected scintillation photons from both excitation and recombination are collectively termed the primary scintillation, or S1. On the other hand, the electrons that escape from the interaction site are drifted towards the liquid-gas interface under the action of an electric field. Upon reaching the liquid surface, a stronger electric field is used to extract the electrons into the GXe, where they induce further excitation and generate more VUV photons by electroluminescence. This delayed signal detected by the same photo-detectors is termed secondary scintillation, or S2. An illustration of an incoming particle from outside a dual-phase xenon TPC interacting with the LXe bulk is presented in Fig 2.1.

The observed S1 and S2 signals offer plenty of information to reconstruct the particle interaction. With adequate calibration, they can be used to measure the energy deposition in the interaction with high energy resolution. Additionally, the partitioning of energy transfer into excitation and ionisation is highly dependent on the primary particle type, making the ratio of S2 to S1 a powerful background rejection tool for analyses such as searching for WIMPs [62]. Moreover, the time delay ΔT between the arrival of the S1 and S2 signals can be used to infer spatial information about the interaction. As the electrons escape from the interaction site, they drift upwards in the electric field at constant velocity v_d . Therefore, the depth z of an interaction can be directly reconstructed from $z = v_d \Delta T$, projecting the spatial information onto the time dimension (“time projection”). Furthermore, the thin layer of GXe in the electroluminescence region means that the S2 scintillation light is highly localised. This makes it possible to infer the lateral position information of the interaction

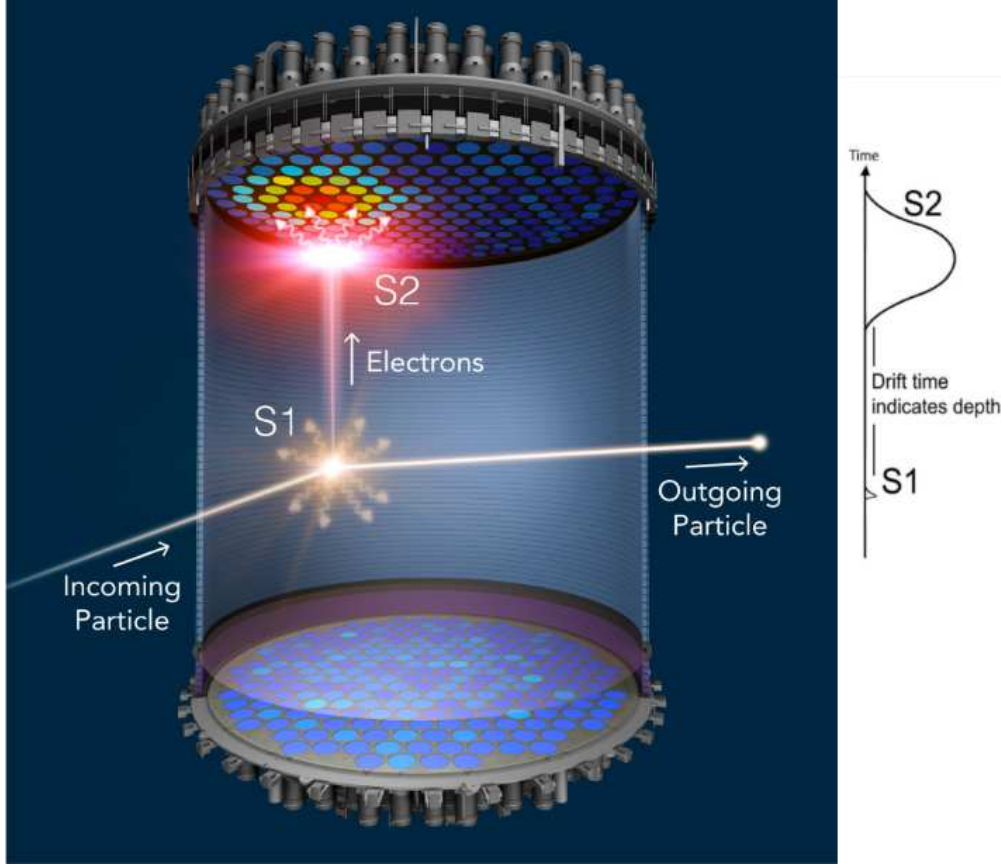


Figure 2.1: Illustration of an incoming particle from outside a dual-phase xenon TPC interacting with the LXe bulk. The interaction deposits energy and subsequent physical processes lead to the production of the S1 and S2 signals. The side plot shows an ideal example of the detected S1 and S2 signals as waveforms, separated apart by the drift time of the electrons. The figure is taken from Ref. [61].

from the hit pattern of light in the array of photo-sensors. By combining this information with the time projection, a full three-dimensional reconstruction of the interaction site can be achieved.

Compared to operating a xenon TPC with only a liquid or gaseous target, a dual-phase TPC takes advantage of amplification of the charge signal in the gas phase, easily providing sensitivity to single ionisation electrons [63]. This property is particularly useful in enhancing the detection efficiency of low energy events, such as the interaction of sub-GeV WIMPs, where the S1 signal falls below its detection threshold. Additionally, the position reconstruction

can all be achieved to a high resolution of $\mathcal{O}(\text{mm})$, allowing for rejection of backgrounds that are expected to have well-defined position dependence or event topology.

While previous and currently operating dual-phase xenon detectors differ in scale, ranging from $\mathcal{O}(10 \text{ kg})$ in the early days to $\mathcal{O}(10 \text{ tonne})$ of LXe in the current generation detectors, the operation of these detectors shares some common experimental configuration. The below list describes such a configuration at a high level, with LZ subsystems described in more detail in Section 2.3:

- Cryogenic cooling systems:** The xenon TPC is typically housed in vacuum insulated cryostat vessels to provide thermal insulation and help to maintain the cryogenic temperature. In LZ, sub-cooled liquid xenon is delivered to the bottom of the detector via a condensation tower external to the detector, where a two-phase heat exchanger provides a large fraction of the cooling power. To maintain the dual-phase condition, xenon inside the TPC needs to be continuously cooled close to its boiling point in the range of $172 - 182 \text{ K}$ at $1.5 - 2.5 \text{ bar}$ [64]. One way to achieve this is to use liquid nitrogen (LN) for cooling through a thermosyphon system. A set of closed-loop vertical thermosyphon heat pipes is attached to the cryostat vessel that houses the xenon TPC, with the other end connected to LN bath above the detector. As the LN flows down the heat pipes, heat is transferred from the cooling element on the cryostat to LN and subsequently boils it off. The N_2 gas then rises up inside the tube, reaching the LN bath and recondenses. As the process continues, xenon inside the cryostat vessel is cooled down and maintained at an equilibrium operating temperature.
- Photo-detectors:** Primary and secondary scintillation light from a particle interaction needs to be measured by photo-detectors. Previous and current generation experiments have used photomultiplier tubes (PMTs) to achieve this, while the usage of novel photo-detectors such as SiPMs in future experiments is under research and development [65]. To improve the light collection efficiency of the detector, the PMTs need to be sensitive to light wavelength in the VUV centred near 175 nm and have a high quantum efficiency [66]. The design of a dual-phase TPC typically has two arrays

of PMTs, one at the top of the GXe region and the other at the bottom of the LXe region. Since the S1 scintillation light is produced isotropically, the wall of the TPC is designed to have high reflectivity for VUV photons to minimise light signal escaping in the transverse direction. In addition, the difference in refractive index between LXe and GXe leads to total internal reflection above some critical angle at the liquid-gas interface, meaning that most of the S1 light is detected in the bottom PMT array. This is in contrast to S2 light, which is produced in the GXe region and is therefore observed mostly by the top PMT array.

- **Electrode grids:** The electric field arrangement in a dual-phase TPC is different for the LXe and GXe regions. A drift field is required in the LXe target to drift the escaped electrons from interaction sites towards the liquid-gas interface region. At the liquid surface, a stronger extraction field is needed to overcome the potential barrier and extract electrons into GXe. The extracted electrons are further accelerated by the electroluminescence field in the GXe region to produce VUV photons. A dual-phase TPC typically has a set of three wire grids, set at different electric potentials to create the electric field arrangement that meets the above requirements. The drift field is created by a cathode at the bottom of the LXe above the bottom PMT array, and a gate grid just below the liquid surface. In LZ the applied voltages generate a drift field strength of $\mathcal{O}(100 \text{ V/cm})$ and drift the electrons at a velocity of $\sim 1 \text{ mm}/\mu\text{s}$. The extraction and electroluminescence fields are created by the gate grid and an anode grid located in the gas a few mm above the liquid surface. As the electrons drift past the gate and reach the liquid level, they experience an extraction field of $\mathcal{O}(\text{kV/cm})$ and enter the GXe region. The strength of the two fields differ by a factor of 1.9 due to the relative dielectric constant of liquid xenon [67]. In LZ there is an additional reverse field region between the cathode and the bottom PMTs, where the direction of the electric field lines is opposite to the rest of the TPC. This is because the bottom PMT array need to operate at near ground potential. To achieve this, the bottom PMT array is surrounded by an extra shield grid at low potential (-1.5 kV in LZ) to protect the PMTs from the high potential of the cathode, thus creating a reverse field

region below. Any escaped electrons from interactions in this region drift away from the GXe, leading to events with only S1 but no S2 signal.

- **Circulation and purification:** Radioactivity in the bulk xenon contributes significantly to the backgrounds for physics searches. Some of these radioactive isotopes can be removed in advance. In LZ this is largely achieved by gas chromatography with cold synthetic charcoal, while other experiments utilise techniques such as cryogenic distillation columns. Another species that requires removal is electronegative impurities, introduced by leakage or outgassing from detector material. They can capture electrons as they drift in LXe and reduce the detector's sensitivity by suppressing the S2 signal. A complex circulation and purification system is needed to obtain a good electron lifetime by continuously removing the impurities. This can be achieved by having a zirconium getter designed as part of the circulation path and passing xenon through it. In LZ the LXe is evaporated before reaching the getter and recondensed after, as the purification process happens more efficiently in the gas phase.
- **Ultralow radiological backgrounds:** Being primarily used for rare event searches, the requirement for ultralow radiological backgrounds applies to most of these subsystems. Tremendous effort (sometimes many years as for the PMTs) has been put in place to search for the right materials and design products with them. This requires comprehensive screening and cleanliness control. For this purpose, LZ has performed an extensive radioassay campaign and designed bespoke quality control and assurance procedure [68].

The TPC transforms particle interactions with the LXe into signal and allows for reconstruction of the events. It is therefore important to understand the physical processes taking place in LXe, in order to reconstruct the events accurately.

2.2 Liquid Xenon Physics

2.2.1 Properties of Xenon

Xenon (Xe) is a noble gas that is chemically very stable. It is an attractive target material for radiation detection and consistently sets world-leading limits for direct detection of weakly interacting massive particles (WIMPs). Table 2.1 summarises the abundance and half-life of naturally occurring xenon isotopes. Most of them are radioactively stable, but some are viable $\beta\beta$ isotopes, making xenon useful for searches of various double beta decay modes. The Standard Model decay modes of the xenon $\beta\beta$ isotopes are ^{134}Xe and ^{136}Xe through double beta decay [3, 69, 70], and ^{124}Xe through double electron capture [71]. The most notable Xe isotope to consider for Majoron-emitting double beta decay searches is ^{136}Xe , which has a natural abundance of about 8.86%. Experiments utilising ^{136}Xe currently set the most stringent limits on the Majoron-neutrino coupling constant for all spectral indices [38, 46].

Table 2.1: Isotopic abundance of natural xenon [72]. The measured half-lives of ^{124}Xe and ^{136}Xe , as well as the current best limit on half-life of ^{134}Xe are obtained from Ref. [69], Ref. [3] and Ref. [71], respectively.

Isotope	Abundance	Half-life
^{124}Xe	0.095%	1.8×10^{22} yrs
^{126}Xe	0.089%	stable
^{128}Xe	1.91%	stable
^{129}Xe	26.4%	stable
^{130}Xe	4.07%	stable
^{131}Xe	21.2%	stable
^{132}Xe	26.9%	stable
^{134}Xe	10.4%	$> 8.7 \times 10^{20}$ yrs
^{136}Xe	8.86%	2.165×10^{21} yrs

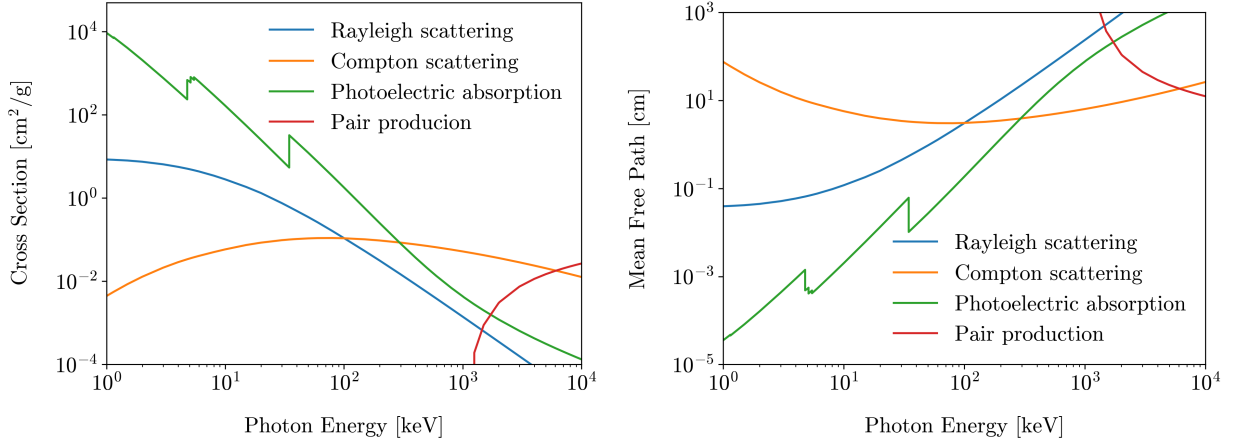


Figure 2.2: The cross section and mean free path of photons in LXe for different electromagnetic processes. Cross section data obtained from Ref. [73] and the mean free paths are calculated accordingly, assuming an LXe density of 3.0 g/cm³.

A detector may be designed to utilise xenon in its gas, liquid, or both phases based on its main scientific goals. Important physical characteristics of xenon that are advantageous for experiments searching for rare events include:

- **Self-shielding:** Liquid xenon has a large atomic mass and liquid density, both of which lead to significant attenuation of radiation. The mean free path of γ ray in LXe depends on the electromagnetic processes involved, which change with energy scales. The common types of photon interactions in LXe include Compton scattering, photoelectric absorption, Rayleigh scattering and pair production. The mean free path of each given electromagnetic process is a function of photon energy as shown in Figure 2.2. Photons with energy below ~ 300 keV are most likely to be absorbed through the photoelectric effect, with a mean free path below 3 cm. At higher energies, Compton scattering becomes the dominant process, increasing the photons' mean free paths to ~ 10 cm. This remains the case up until ~ 6 MeV, where pair production becomes the dominant process. This property of being a strong attenuator of photons means that detectors with a large mass of LXe can shield external γ ray, leaving a relatively quiet central volume with very low backgrounds, especially at low energies.

In comparison, electrons lose energy rapidly in LXe from excitation and ionisation, nuclear (Rutherford) scattering and bremsstrahlung emission. A typical 1 MeV electron in $0\nu\beta\beta\phi$ search has a range of ~ 2 mm in LXe [74], which is well below the typical range of γ ray.

- High signal yields:** Energy deposition of particle interactions in LXe produces detectable signals in the form of scintillation (light) and ionisation (charge). The light and charge yields are affected by the electric field applied to LXe, the energy deposition, and the type of interacting particle. A typical detector condition of $\mathcal{O}(100 \text{ V/cm})$ electric field in a dual-phase xenon TPC generally gives very efficient light and charge production. An electron interaction with energy deposition of 1 MeV on average produces $\sim 3 \times 10^4$ scintillation photons [75]. Also, the energy required to produce an electron-ion pair (the ionisation W -value) in LXe is relatively low at about 14.3 eV [76]. The same 1 MeV electron produces $\sim 7 \times 10^4$ ionisation electrons, most of which can be extracted into the gas phase and generate $\sim 4 \times 10^7$ electroluminescence photons. Detecting both the scintillation and ionisation signals enable one to perform energy and position reconstruction of the interaction to a high level of accuracy and precision. It is worth noting that there is an anti-correlation between light and charge yield for the majority of energy range of interest for double beta decay, since electrons either escape the primary track and contribute to S2 or they recombine and contribute to S1. When performing energy reconstruction, the anti-correlation essentially cancels out some statistical uncertainties in the yields event-by-event, enabling one to achieve an energy resolution value σ/E as low as 0.67% at the 2.46 MeV Q-value of ^{136}Xe [1]. This is of great importance to an experiment's ability to search for physical processes with mono-energetic signals, such as $0\nu\beta\beta$. The ratio between light and charge yields is also affected by the ionising particle and the interaction type, providing a sensitive signal-background discrimination tool with $> 99.5\%$ efficiency in WIMP searches [77].
- Radioactively stable:** Xenon at natural abundance has a low intrinsic background rate. The only radioactively unstable isotopes are ^{124}Xe , ^{134}Xe and ^{136}Xe , all of which are $\beta\beta$ isotopes whose standard model decay modes are highly suppressed and have

long half-lives. For WIMP experiments, this means intrinsic activity from the LXe target only becomes a significant background source in large tonne-scale experiments. For double beta decay searches the picture is different, given that the unstable Xe isotopes are now both the background and the signal source. Nevertheless, the aforementioned self-shielding property can still simplify the situation by providing a quiet central volume where external backgrounds are shielded and therefore subdominant compared to the intrinsic activity of the Xe isotope of interest.

2.2.2 Particle Energy Transfer to Liquid Xenon

A particle interaction with LXe can be generally categorised into either an *electron recoil* (ER) or a *nuclear recoil* (NR). ER happens when the incident particle interact with the electrons of the atom, while NR takes place when the incident particle elastically scatters with the xenon nucleus. For a $0\nu\beta\beta\phi$ search, almost all interactions to be considered are ER events. The two interactions types have some differences in the corresponding scintillation and ionisation mechanisms. This section focuses on the mechanisms for ER, unless otherwise indicated. A comprehensive review of the scintillation and ionisation mechanisms for both interaction types can be found in Ref. [59].

A particle interaction in LXe can deposit energy via three separate forms: excitation, ionisation and heat. For electrons, partitioning of the total energy deposition E_0 into these processes is described by the Platzman equation [78]:

$$E_0 = N_{ex}E_{ex} + N_iE_i + N_i\epsilon, \quad (2.1)$$

where N_{ex} and N_i are the number of excited atoms and the number of ion-electron pairs; E_{ex} and E_i are the average energies required for excitation and ionisation of an atom to take place; and ϵ is the mean energy below which free electrons only participate in elastic scatterings with atoms and deposit energy as heat. Excited atoms produce (indirectly) scintillation photons and the external electric field extracts a fraction of the ionised electrons, leading to two observable signals: light and charge.

A naive interpretation of the detectable signals would be that all the N_i electrons contribute to the charge signal, while the light signal comes solely from excitation. However, this simple picture is complicated by the presence of recombination of ion-electron pairs. Not all electrons from ionisation are extracted from the pairs by the external electric field. In fact, a sizeable proportion of the N_i ion-electron pairs recombine and produce additional scintillation photons, leading to an enhanced light yield. This also gives an event-by-event anti-correlation between light and charge yields, which is very useful when considering event energy reconstruction. A strong external electric field helps to reduce the recombination probability and increase the charge yield. Other factors including the particle's ionisation density and the resulting track structure also affect recombination probability [62]. For example, electrons have low ionisation density (i.e. dE/dx) and recombination only takes place if the ionised electrons are within the Onsager radius, whereas α particles produce much denser tracks with higher recombination probability. Since the ionisation density of a particle is a function of its energy, the light and charge yields are both energy dependent. Other than recombination, the type of interaction also affects the light and charge yields. ER and NR have very distinct excitation to ionisation ratio N_{ex}/N_i , with the value sitting in the range 0.06–0.2 for ER and close to unity for NR [79–81].

In the context of a dual-phase xenon TPC, the actual value of N_{ex} and N_i from an interaction cannot be directly measured. Instead, they are inferred from observation of the light and charge signals, thus allowing calculation of the energy transfer E_0 . Scintillation photons from both the initial excitation and from recombination contribute to the light yield. These photons are detected promptly after the interaction and the signal is termed *primary scintillation*. On the other hand, the charge yield measurement comes solely from the electroluminescence light from extracted electrons in the gas phase. As the electrons take time to drift towards the gas phase, there is a delay in detection of the corresponding signal.

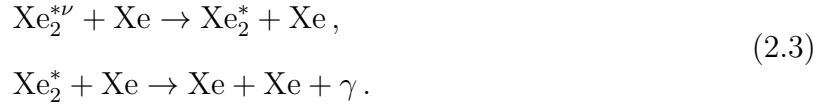
2.2.3 Primary Scintillation

Particle interactions in LXe lead to emission of scintillation photons with a peak wavelength of 175 nm in the vacuum ultraviolet (VUV) range. Rather than direct relaxation of an

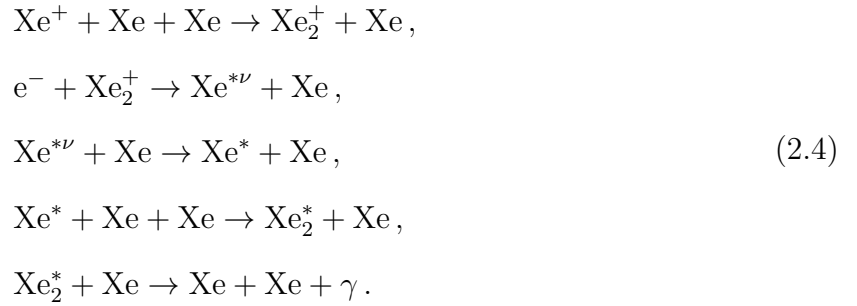
excited atomic state, the relaxation actually comes from an excited diatomic molecular state Xe_2^* . For the initial excitation, an ionising particle A interacts with a Xe atom via the following process:



where the superscript ν denotes a diatomic molecule in an excited vibrational state, whose relaxation to its ground state occurs through collision rather than radiation; and the superscript $*$ denotes an excited electronic state and the subsequent relaxation is radiative. As the relaxation emits a scintillation photon γ , the diatomic molecule dissociates:



A scintillation photon from the recombination process is produced via a different set of steps:



While both excitation and recombination lead to scintillation photons of the same wavelength of 175 nm, there are still subtle differences in the products of the two processes. Scintillation photons come from radiative decay of one of the two excited molecular states, the $^1\Sigma_u^+$ singlet state with a lifetime of 2–4 ns, or the $^3\Sigma_u^+$ triplet state with a lifetime of 21–28 ns [82][83]. For ER there is a non-exponential third component of scintillation with a lifetime of 30–45 ns [84] as a result of the thermalisation time of electrons in recombination. This component is suppressed by electric field and disappears completely at a few kV/cm, supporting the interpretation of its recombination origin. For a typical 1 MeV electron energy, all three components contribute to the ER scintillation timing. It has also been observed that particles such as high energy electrons tend to populate the triplet states, while those with high dE/dx tend to populate singlet states. This difference in relative population

of singlet and triplet states renders an observable difference in the pulse shape, providing a method of particle identification which can be effective at higher energies [77].

The efficiency of photon production in primary scintillation is measured by the light yield $L_y = N_{ph}/E_0$, where $N_{ph} = N_{ex} + rN_i$ is the total number of photons produced in an interaction with a probability of recombination r . The recombination process conserves the total number of quanta, therefore the following relationship holds:

$$N_{ph} + N_e = N_{ex} + N_i. \quad (2.5)$$

An alternative measure of efficiency of light production is to consider the average energy required to produce one scintillation photon. This is the reciprocal of the light yield and is termed the scintillation W -value, $W_{ph} = E_0/N_{ph}$. In older literature a similar but distinct ionisation W -value, $W_i = E_0/N_i$ is often quoted, measuring the average energy required to produce an ion-electron pair, rather than scintillation photon. Scintillation photon production is the most efficient when no external electric field is applied and practically all ion-electron pairs recombine (assuming no further quenching effect):

$$W = \frac{E_0}{N_{ex} + N_i} = \frac{W_i}{1 + N_{ex}/N_i}. \quad (2.6)$$

Both the excitation to ionisation ratio N_{ex}/N_i and the ionisation W -value are independent of energy [80], so W is a constant. The value of W is taken to be 13.5 eV [85], between recent measurements [62, 86]. For the remainder of this thesis, the word “ W -value” refers to W unless otherwise specified. This offers a simple energy reconstruction formula, relating energy deposition and the number of quanta produced from an ER interaction:

$$E_0 = W(N_{ex} + N_i) = W(N_{ph} + N_e). \quad (2.7)$$

The implication of Eq. 2.7 is that if both the light and charge signals are observed, energy reconstruction of an ER interaction can be performed event-by-event, intrinsically taking recombination into account. Moreover, this type of energy reconstruction results in a better energy resolution, as the anti-correlation between light and charge signal essentially removes the recombination fluctuations, which are very variable with track topology.

There is a further complication to energy reconstruction for nuclear recoils. As the particle scatters elastically with the Xe nucleus, the whole atom recoils and interacts with the nearby atoms. As a result, a fraction of the energy is transferred into heat that does not produce any detectable signal. This fraction can be estimated using the theory of Lindhard [81], and the energy reconstruction formula for nuclear recoils requires an additional Lindhard quenching factor $\mathcal{L}$:

$$E_0 = \frac{W}{\mathcal{L}}(N_{ph} + N_e). \quad (2.8)$$

A fraction of the N_{ph} photons are eventually converted to electronic signals by photodetectors such as photo-multiplier tubes (PMTs). The measured primary scintillation signal, denoted S1, is given by:

$$S1 = g_1 N_{ph}, \quad (2.9)$$

where the unit of S1 is the number of photons detected (phd) and g_1 is the photon detection efficiency of the detector, taking into account the quantum efficiency of the PMTs, the geometrical light collection efficiency and other factors. A typical range of g_1 for a dual-phase xenon TPC is 0.05 – 0.15 phd/photon.

2.2.4 Ionisation Charge

In a dual-phase TPC, ionisation electrons that escape the recombination process are drifted by the electric field towards the liquid-gas interface. They then get extracted into the GXe region, where they collide with xenon atoms to produce Xe_2^* excited states under the strong electric field of $\mathcal{O}(10 \text{ kV/cm})$, producing further electroluminescence. Photodetectors such as PMTs then convert the scintillation photons into an electronic signal, denoted S2, which has a certain time delay from the primary scintillation signal.

The electrons have a constant drift velocity of $v_d \sim 1 \text{ mm}/\mu\text{s}$ under the action of an $\mathcal{O}(100 \text{ V/cm})$ electric field. For a multi-tonne-scale experiment, this is equivalent to a maximum electron drift time of hundreds of microseconds. During this drift time Δt , the spatial distribution of the electron cloud evolves under diffusion, with a spread of:

$$\sigma_{L,T} = \sqrt{2D_{L,T}\Delta t}, \quad (2.10)$$

where the subscripts L and T refers to diffusion in the longitudinal and transverse direction, respectively. The longitudinal diffusion component leads to a time spread for electrons to be extracted in the the GXe region. An event from the bottom of the detector has an observed S2 pulse with a shape close to Gaussian. Since the coordinate reconstruction of an interaction is projected onto the time dimension in a TPC, a spread in pulse arrival time reduces the longitudinal position resolution of the detector. This has a significant impact on the detector's ability to distinguish signal and background events based on event topology, such as Compton scattering of γ rays that deposit energy at multiple interaction sites. The measured values of D_L and D_T (at ~ 200 V/cm) are ~ 25 cm²/s [87] and ~ 55 cm²/s [88], respectively.

In addition to the basic near-Gaussian component, the S2 pulse shape may be complicated by other physical processes. It is speculated that as the drift electrons arrive at the liquid-gas interface, the large potential barrier between the two phases traps a population of the drift electrons for time periods of $\mathcal{O}(10$ ms) before they get extracted into the GXe region [89]. There is an even slower component of the S2, arising from the release of captured electrons by electronegative impurities. Both of these delayed components of the S2 signal have an arrival time period that can be much longer than the typical event window in a dual-phase TPC, and they are especially important at the relatively high energies involved in a $0\nu\beta\beta\phi$ search. Possible adverse effects include triggering the data acquisition system to record the delayed part of the S2 pulse as a separate signal, or show up as a long trail after the main S2 pulse. The latter is much more important in practice as it is sometimes difficult to identify where the main S2 ends and the tail begins. For multiple scatters, the second S2 pulse can even hide the tail. The presence of the long tail hinders the energy resolution for both single and multiple scatters.

As mentioned previously, the presence of electromagnetic impurities (e.g. O₂) in the LXe can capture drift electrons on their path to the GXe region. This leads to a diminishing number of drift electrons reaching the liquid-gas interface which depends on drift time:

$$N_e = N_e^0 e^{-\Delta t/\tau}, \quad (2.11)$$

where N_e^0 is the initial number of electrons and τ is the free electron lifetime. In order to reduce the attenuation of drifting electrons, detectors require circulation and purification systems designed to constantly remove impurities. An electron lifetime of 5–8 ms can be achieved with current generation multi-tonne-scale experiments [53], which is significantly longer than the maximum drift time in the TPC and is ample for the detection efficiency of small signals.

One of the main advantages of having a GXe electroluminescence (EL) region is the amplification effect to light per unit charge. The EL yield is related to the pressure and the electric field in the GXe region through an empirical formula:

$$\frac{dN_{EL}}{dx} = \alpha E - \beta P - \gamma, \quad (2.12)$$

where the values of the parameters can be found in Ref. [59]. Under typical detector conditions, with a pressure of 1.6 bar and a gate-anode potential difference of 10 kV, the EL yield is of $\mathcal{O}(1000 \text{ photons/cm})$. This amplification in charge signal means that a dual-phase TPC is sensitive to even single electrons and therefore have very low energy threshold.

The EL photons are again detected by PMTs and converted to a second electronic signal S2 in units of photons detected:

$$S2 = \varepsilon g_1^{gas} N_{EL} N_e = \varepsilon \langle SE \rangle N_e = g_2 N_e, \quad (2.13)$$

where ε is the extraction efficiency of electrons at the liquid surface, g_1^{gas} is the light detection efficiency in the gas phase, $\langle SE \rangle$ is the average number of photons detected from a single electron, and g_2 is the overall gain factor. Combining Eq. 2.7, Eq. 2.9, and Eq. 2.13, one can write the energy reconstruction formula for electron recoils in terms of the observed S1 and S2 signals:

$$E_0 = W \left(\frac{S1}{g_1} + \frac{S2}{g_2} \right). \quad (2.14)$$

2.3 The LUX-ZEPLIN (LZ) Experiment

LZ is a dual-phase xenon TPC experiment with the primary scientific goal of searching for WIMPs. The LZ collaboration was formed by groups participating in the previous generation LUX and ZEPLIN-III experiments. The LZ detector is located in the Davis Campus at the 4850-ft level of the Sanford Underground Research Facility (SURF) in South Dakota, USA, where the previous LUX experiment had been installed. At the time of writing, LZ has published its first dark matter search results based on the first science run (SR1) of the experiment. The results have set the most stringent limits for spin-independent WIMP-nucleon scattering cross section to date, as well as for the WIMP-neutron spin-dependent interactions [53].

Table 2.2: Parameters of the LZ detector as reported in its first dark matter search result [53].

Parameter	Value
TPC diameter	145.6 cm
LXe temperature	174.1 K
GXe pressure	1.791 bar
Drift field in LXe	193 V/cm
Extraction field in GXe	7.3 kV/cm
Maximum drift time (length)	951 μ s (145.6 cm)
Electron lifetime	5000–8000 μ s
g_1	0.114 $\pm$ 0.002 phd/photon
g_2	47.1 $\pm$ 1.1 phd/electron

A schematic of the LZ experiment is shown in Figure 2.3. At its core, LZ utilises a dual-phase xenon TPC that contains 10 tonnes of LXe, 7 tonnes of which is active and act as the target material. The TPC is mounted in a double-walled titanium cryostat, with the inner cryostat vessel (ICV) suspended inside the outer cryostat vessel (OCV), made of ultra-low activity titanium [90]. A set of three pipes is installed in the vacuum space between the two vessels for delivery of radioactive sources for calibration. Between the TPC and the

ICV wall, there are regions filled with LXe that is not considered part of the active LXe target. These regions are monitored by PMTs attached to the TPC and the ICV wall and is collectively referred to as the xenon skin. A set of 10 acrylic vessels containing 17 tonnes of gadolinium-loaded liquid scintillator (GdLS) surrounds the cryostat, forming the outer detector (OD). The OD is observed by an additional set of PMTs immersed from a stand-off distance. The xenon skin and the OD provides additional detector systems to the TPC itself and act as anti-coincidence vetoes. The entire LZ detector system stands inside the Davis Campus water tank, containing 238 tonnes of ultra-pure water to provide shielding from neutrons and γ rays. Table. 2.2 list some of the main detector parameters of LZ at the time of publication of its first results.

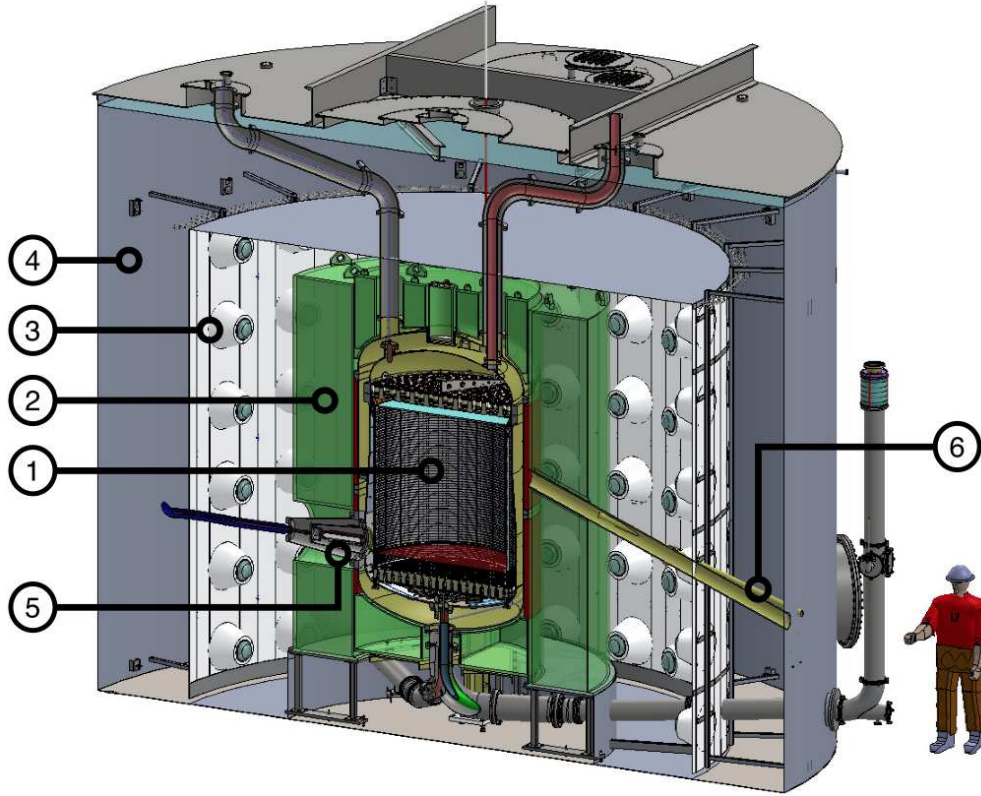


Figure 2.3: Schematic of the LZ detector design. The labelled subsystems are the liquid xenon TPC (1), the OD acrylic vessels filled with GdLS (2), the 8-inch PMTs observing the OD (3), the water tank (4), the cathode high voltage connection (5) and the conduits for neutron calibration (6). This figure is taken from Ref. [91].

2.3.1 Detector Design

TPC

The centre of the LZ detector system is the cylindrical xenon TPC. A schematic of the LZ TPC is shown in Figure 2.4, and a photo of the assembled TPC is shown in Figure 2.5. It has a drift region with 145.6 cm in diameter and 145.6 cm between the cathode and gate, housing 7 tonnes of active LXe target. Above the LXe there is a thin layer of GXe with thickness of 8 mm, and below the cathode grid there is an LXe-filled reverse field region (RFR), terminating 13.7 cm away from the cathode. The xenon volumes are contained between two arrays of PMTs at the top and bottom, and surrounded by the TPC field-cage from the side. The field-cage is made with polytetrafluoroethylene (PTFE) panels that are highly reflective (over 97%) for the VUV scintillation light, increasing g_1 as much as possible [92].

There is a total of 494 Hamamatsu 3-inch R11410-22 PMTs in the TPC, 241 on top array and 253 on bottom array. This PMT model is similar to that used by other LXe experiments but the 22-variant was tuned specifically for LZ. The PMT model has an average quantum efficiency (QE) of 30.9% [93] for detecting the 175 nm VUV scintillation light at the LZ operating temperature. The PMTs operate at an average gain of 2×10^6 . The two PMT arrays also have distinct spatial arrangement to optimise position reconstruction of events close to the TPC wall. The top array is arranged in a hybrid pattern with hexagonal pattern near the centre and circular pattern near the edge. The bottom array is arranged in a purely close-packed hexagonal pattern.

Xenon Skin

The xenon Skin refers to the region between the outer walls of the TPC field-cage and the ICV, containing more than 2 tonnes of LXe that is not considered as part of the active volume. The region is further divided into two main sub-volumes: a “side Skin” volume outside the TPC field-cage, and a “dome Skin” region below the bottom PMT array. The xenon Skin provides dielectric standoff between the biased TPC components and the grounded ICV, but

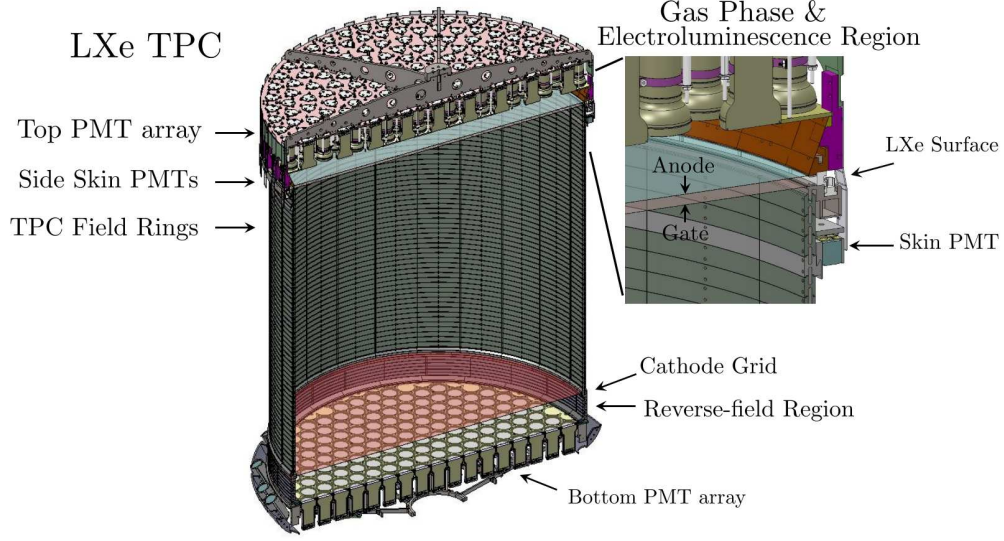


Figure 2.4: Schematic of the LZ TPC. The xenon volumes are surrounded by the TPC field-cage from the side, and viewed by the top and bottom PMT arrays. The right insert zooms in on the gas phase and electroluminescence region, where the S2 signal generation occurs. This figure is adapted from Ref. [61].

also acts as an anti-coincidence veto detector for background rejection.

Because of the high density of LXe, the Skin is particularly effective at detecting γ ray interactions within the region. These γ rays mainly originate from radioactive isotopes in detector materials, with a small contribution from the external cavern rocks. Neutrons may also scatter in the Skin region, albeit to a lesser extent. If scintillation light is observed in both the TPC and the Skin within a very short time window, the event is most likely to be a multiple scatter background, thus providing an anti-coincidence veto for data analysis. In addition, light leakage from the Skin into the TPC may result in a larger than expected S1 signal and compromises the particle discrimination based on the S2 to S1 ratio. It is therefore essential to instrument the Skin to monitor such activities. The Skin is also capable of tagging spurious light emission, which may occur due to high voltage.

The Skin has uneven thickness from top to bottom due to the tapered ICV shape visible in Figure 2.3. The side Skin is just 4 cm thick at the top but widens to 8 cm near cathode

level for adequate standoff. There are 93 Hamamatsu R8520 1-inch PMTs in the top half of the side Skin, located just below the LXe surface and viewing down. The bottom half of the side Skin is instrumented with 20 R8778 2-inch PMTs viewing up the region. There are 18 further R8778 PMTs mounted below the bottom array to monitor the dome region.

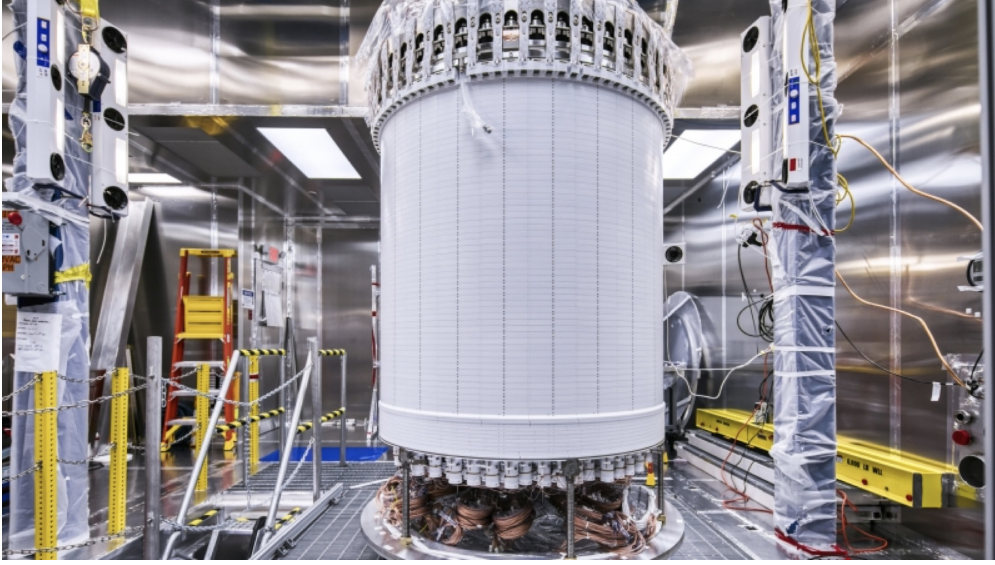


Figure 2.5: The assembled LZ TPC. This photo was taken by Matthew Kapust, Sanford Underground Research Facility.

Outer Detector

The outer detector (OD) system immediately surrounds the OCV. The OD is composed of a set of acrylic vessels (AVs): four large ones that surround the side of the cryostat, and seven smaller ones at the top and bottom. In total, the AVs are filled with $\sim 17,000$ kg of GdLS. The liquid scintillator is based upon a linear-alkylbenzene (LAB) solvent, loaded with 0.1% Gd by mass. The scintillator is treated with additional purification to reduce uranium, thorium and potassium impurities [61]. The huge (n, γ) cross section (49 kb) of natural Gd allows the OD to detect neutron interactions efficiently. Neutrons are predominantly captured by ^{155}Gd and ^{157}Gd , releasing a cascade of γ photons with a total of 7.9 MeV and 8.5 MeV respectively. There is also $\sim 10\%$ of neutrons captured by hydrogen, emitting a single 2.2 MeV γ photon in the process. In addition, γ rays from detector materials and from the laboratory rock may also deposit energy in the GdLS.

Scintillation light produced in the GdLS is detected by 120, 8-inch Hamamatsu R5912 PMTs, arranged in 20 rings of evenly spaced groups of 6. The PMTs are immersed in water, all mounted on metal ladders that also hold a Tyvek reflector curtain that is 115 cm radially away from the side AVs. The OD is designed to optimise for a high neutron detection efficiency, to support the primary WIMP-search mission of the experiment. For TPC single scatters in the NR band, a position-averaged neutron tagging efficiency of $89 \pm 3\%$ has been achieved [53]. For γ ray backgrounds that are more relevant for $0\nu\beta\beta\phi$ searches, the typical TPC and OD signals are essentially coincident within a narrow time window.

Water Tank

LZ uses the same Davis Campus water tank that formerly hosted the LUX experiment [94]. The water tank is cylindrical in shape, with a height of 5.9 m and a radius of 3.8 m. It is filled with 238 tonnes of ultra-pure water, providing shielding against external background sources including γ rays and neutrons from the cavern rock, as well as those from muon interactions. The water is purified to achieve a maximum acceptable level of 2 ppt, 3 ppt and 4 ppb for uranium, thorium and potassium impurities, respectively [94].

2.3.2 Calibrations

LZ is designed to accommodate extensive calibrations throughout its lifetime. Many of these calibrations have already been conducted during the data taking leading up to its SR1 result [53], with the others planned for future calibration campaigns. This work will mention some of the most relevant ones to set the context of data analysis. An extensive list of the calibration sources planned for LZ can be found in Ref. [91].

Several calibration sources are gaseous in natural conditions. Such sources are typically injected into GXe during circulation, thus dispersed into the active region. Important quantities coming out of these calibrations include S1 and S2 uniformity corrections, responses to ER and electron lifetime determination. As an example, ^{131m}Xe decays via 164 keV γ ray

emission with a half-life of 11.9 days. This short half-life ensures that the source does not contaminate the active xenon for too long. Another commonly used source is ^{83m}Kr , with signature conversion electron emissions at 32.1 keV and 9.4 keV. Its short half-life of 1.83 hours was sufficient in past experiments for uniform dispersion. However, for multi-tonne-scale experiments many decays will occur before the source becomes uniformly distributed. Nevertheless, it still provides useful calibrations for S1 and S2 detector responses, as well as a tool for tagging the spatial flow of xenon during circulation. LZ also deploys tritiated methane (CH_3T); tritium is a beta emitter with a 18.6 keV endpoint, in order to understand detector responses to low energy ER events. This source has a long half-life of 12.5 years and must therefore be efficiently removed by the getter to prevent long-term contamination.

As part of the detector design, there are 3 small-diameter source tubes in the vacuum region between ICV and OCV. The purpose of these tubes is for easy delivery and removal of samples of external radioactive sources into the detector for calibrations. For example, synchronisation of the TPC, skin and OD can be calibrated by deploying ^{22}Na down the tubes and observe the two back-to-back 511 keV γ rays. A very important calibration source, especially for double beta decay searches, is ^{228}Th . The 2,614 keV γ ray emission from the ^{208}Tl daughter in the decay chain lies closely to the 2,458 keV Q-value of ^{136}Xe . It is therefore common practice to use this γ ray line as a reference in energy reconstruction calibrations, as well as measuring the energy resolution and hence estimate the expected performance at the Q-value. Calibrations on higher energy nuclear recoil (NR) responses are conducted by directing 2.45 MeV neutrons from a deuterium-deuterium (DD) generator to the cryostat side, collimated through the narrow part of a (bifurcated) neutron conduit. A deuterium-based reflector is placed behind the DD generator to collect reflected neutrons and convert them into a quasi-monoenergetic (minimum energy 272 keV) neutron beam, which is then directed to the cryostat side through the wide part of the neutron conduit. For very low nuclear recoil energy up to 4.6 keV, a range that corresponds to ^8Be solar neutrino coherent scattering, calibration relies on the YBe photoneutron (γ, n) source which can be transported to the cryostat top via a large-diameter guide tube.

2.3.3 Signal Processing and Data Acquisition

The LZ signal processing electronics is optimised for low energy WIMP interactions, requiring a single photoelectron (SPE) detection efficiency of at least 90% [91]. Analog signals from the PMT systems are transmitted to detector breakouts, subsequently processed by a set of amplifiers and conditioned by front-end amplifiers outside the water tank. LZ amplifiers provide dual-gain outputs with low gain (LG) and high gain (HG) on the pulse-area at 4 and 40, respectively. The main motivation to include an LG mode is to reduce electronics saturation from larger S2 signals and obtain accurate reconstruction of higher energy events, while still maintaining an adequate SPE detection efficiency which is vital for WIMP searches. All TPC, Skin and OD PMTs use the same dual-gain amplifiers but the Skin PMTs only operate in HG mode, while the TPC and OD PMTs use dual-gain signal processing.

The amplifiers are connected to DDC-32 digitisers, digitising the amplified PMT signals at 100 MS/s sampling frequency and 14-bit resolution [95]. The DDC-32s operates in a pulse-only digitisation (POD) mode that reduces the raw waveform volume and thus storage requirements. It is a zero-suppression method that only starts and ends the digitisation when the PMT signal rises above or falls below certain thresholds. In addition, a set number of samples before and after the threshold crossings are also recorded to capture a full pulse. The mode reduces the number of waveforms being digitised and the resulting waveforms are referred to as PODs. Using the built-in S1 and S2 filters, the digitisers are able to detect S1 and S2-like pulses based on pulse shape and the multiplicity vectors of groups of PMTs. The triggering system uses the pulse information to select events of interest and send trigger signals to the data acquisition (DAQ) system. Triggering can be based on S1s only, S2s only or requiring both S1s and S2s. During LZ's SR1 WIMP search, the DAQ operated in S2 mode and recorded an event time window of 2 ms before and 2.5 ms after the S2 trigger.

2.3.4 Data Flow and Data Storage

A schematic of the LZ data flow is shown in Figure 2.6. The digitised data from the DAQ are sent to local Data Collector disks, DAQ1–DAQ15. From there, the relevant information

are extracted by five Event Builders (EB) and stored on the 16 TB local disk array at each EB, before getting transferred to the 192 TB RAID array installed on the SURF surface. The raw data files are then distributed to data centres and processed for offline data analysis.

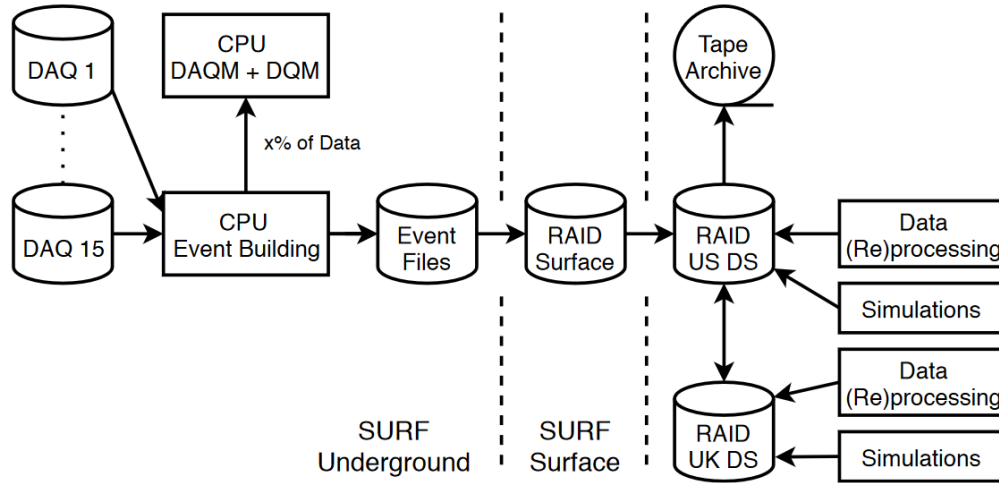


Figure 2.6: Schematic of the LZ data flow. This figure is taken from Ref. [91].

LZ has two data centres, one in the US and one in the UK. The National Energy Research Scientific Computing (NERSC) centre at LBNL acts as the US data centre (USDC), while the UK data centre (UKDC) is located at Imperial College London. Both data centres are capable of storing, processing, simulating and analysing the LZ data. The two data centres act as backup for each other and share the load of data access and processing. The raw data files are sent from the SURF surface to the USDC, then relayed to the UKDC, in order to avoid bandwidth limitation at SURF. Subsequent processing of data can happen at one or both of the data centres, and newly generated data files at one centre are copied over to the other. At the time of this work, the accumulated LZ data is around 7 PB.

2.3.5 Simulation and Data Analysis Framework

A comprehensive set of software tools were developed for analysis of LZ data. These include simulation of detector physics and signal processing electronics, signal reconstruction software, and custom data analysis software for end-users. Together, the data analysis framework enables a complete workflow for analysts to understand the detector response and advance

in physics interpretation of LZ data.

The full detector geometry of LZ has been simulated with BACCARAT, which utilises the GEANT4 toolkit to track particles and identify their interaction points [96, 97]. As illustrated in Figure 2.7, the simulation then splits into two separate chains: the full chain that enables a complete optical simulation of light and charge produced in interactions, and the fast chain that only records energy deposits. The full chain passes photon PMT hits recorded by BACCARAT to Detector Electronics Response (DER), which applies specific PMT effects such as dark counts, quantum efficiency and dual photoelectron response. The DER also simulates electronics response and translates BACCARAT output into waveforms. The DER output is organised in a similar format as real data, allowing for them to be passed through the event analysis framework. In contrast, the fast chain passes the recorded energy deposits through the Noble Element Simulation Technique (NEST) library [75]. NEST applies parametric models to generate S1 and S2 signals.

In the case of both full chain simulation and real data, the output waveforms are processed by the LZ Analysis Package(LZap), where pulse finding and classification algorithms are applied to reconstruct the event. At this stage, corrections on quantities such as S1 and S2 areas are also applied based on position dependent yields. The outputs of LZap are referred to as reduced observable quantities (RQs), which allows for analysts to interact with and apply analysis cuts for physics interpretation. The fast chain simulation does not go through LZap, and the RQs are obtained directly from NEST outputs. However, given that NEST results rely on detector-averaged quantities and lack the information of photon PMT hits, it can only output a limited subset of observable quantities compared to the full chain.

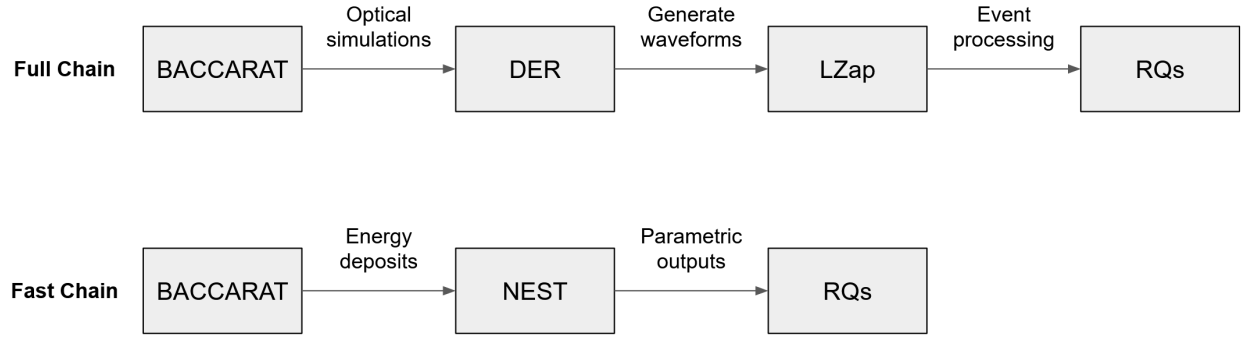


Figure 2.7: Schematic of LZ simulation chains. At the top of the figure is the full chain with accurate simulation, leading up to event-level analysis. The bottom is the fast chain with high statistics, leading up to sensitivity analysis.

Chapter 3

Projected Sensitivity of LZ to Majoron-Emitting Modes of ^{136}Xe

LZ is primarily designed for the direct detection of WIMPs, but the scale of the experiment enables it to search for many other physical phenomena, including $0\nu\beta\beta\phi$ in ^{136}Xe . Assuming natural abundance, the active LXe volume contains more than 600 kg of ^{136}Xe . This compares favourably with the previous generation of dedicated double beta decay search experiments that use enriched xenon, such as EXO-200 and KamLAND-Zen. While the low-background construction of LZ was mostly optimised for $\mathcal{O}(\text{keV})$ WIMP scatters, it does have a much lower energy threshold than many dedicated double beta experiments and allows for a more complete coverage of the $0\nu\beta\beta\phi$ energy spectrum. In addition, LZ has the advantage of significant self-shielding and a large exposure of ^{136}Xe due to its scale. All of these features allow for LZ to competitively search for $0\nu\beta\beta\phi$ in ^{136}Xe .

This chapter discusses the different steps required to reach the projected sensitivity of LZ to $0\nu\beta\beta\phi$ in ^{136}Xe based on simulations. The chapter begins with an overview of the search strategy for the $0\nu\beta\beta\phi$ signal. This is followed by some extended discussion on the LZ simulation framework and an introduction to major background sources. Monte Carlo simulations of $0\nu\beta\beta\phi$ events are generated and the expected LZ detector response to these events is analysed. With both the signal and background simulations available, the fiducial volume (FV) and region of interest (ROI) for the search are optimised. The background model

within the optimised FV is then informed from simulation with estimated background rates for each source. Finally, a likelihood-based analysis is performed to assess the projected sensitivity of LZ to $0\nu\beta\beta\phi$ over a conservative 500 days of livetime.

3.1 Search Strategy

The search strategy for ^{136}Xe $0\nu\beta\beta\phi$ is to look for an excess of events within a region of interest (ROI) in the reconstructed energy spectrum compared to the background model. The observable energy deposition of a $0\nu\beta\beta\phi$ event comes entirely from the two electrons, with the emitted Majoron carrying away “missing energy” from the detector. Because $0\nu\beta\beta\phi$ events form an energy continuum, the ROI is not strictly defined and is subject to optimisation based on other analysis cuts applied to data, which will be discussed in further detail in Section 3.5. The success of the search relies on accurate energy reconstruction of the events, background rejection techniques, and understanding of the background activities.

The electrons emitted in the $0\nu\beta\beta\phi$ event interact with the LXe detector via electron recoils (ER). As will be discussed in Section 3.3, the majority of $0\nu\beta\beta\phi$ events will be reconstructed as single scatter interactions. These events have a single S1 signal paired with one S2 signal. This simple event topology allows for the position coordinates of the interaction to be determined. The two-dimensional x, y coordinates can be obtained from position reconstruction with the Mercury algorithm, based on individual “light response functions” measured for each PMT *in situ*, with detailed implementation found in Ref. [98, 99]. The depth of the interaction can be projected from the difference in time arrival of the S1 and S2 signal. It is expected that the position resolution of x, y is $\mathcal{O}(10\text{ mm})$ and that in the z -direction is $\mathcal{O}(1\text{ mm})$. The three-dimensional position reconstruction also enables position-based corrections to S1 and S2 signals, in order to obtain a uniform response throughout the active region and hence better energy resolution [53].

The combination of the two signals also enables energy reconstruction of the event following a similar formula as Eq. 2.14. One important caveat that has long been known is that for

events with energy of $\mathcal{O}(100 \text{ keV})$ or higher, the amount of light seen in most PMT channels in the top array are large enough to cause amplifier and digitiser saturation, resulting in under-reporting of the size of the S2 signal. One way to reduce this saturation effect is to use only S2s from the bottom array. Together with the correction factors applied to the S1 and S2 signals, the energy reconstruction formula adopted for the purpose of $0\nu\beta\beta\phi$ searches is thus:

$$E = W\left(\frac{S1_c}{g_1} + \frac{S2_{c_{bot}}}{g_{2bot}}\right), \quad (3.1)$$

where the W-value has the same physical meaning as in Eq. 2.14 and has an assumed value of 13.5 eV [85], the c denotes the position-corrected S1 and S2 signals, and the subscript “bot” refers to bottom array-only quantities. The values of g_1 and g_{2bot} are determined from SR1 data to be 0.1136 ± 0.0020 phd/photon and 14.89 ± 0.48 phd/electron respectively [53].

The predominant single scatter (SS) reconstruction of the $0\nu\beta\beta\phi$ events also provides a strong observable to reject background events. Some of the major ER background sources come from outside the LXe, such as γ rays from detector materials or the cavern wall. The high-energy γ rays can scatter multiple times in LXe, resulting in the event being reconstructed as a multiple scatter (MS) interaction. Therefore, restricting the analysis to only events that are reconstructed as SS significantly reduces such backgrounds, while retaining the majority of signal events.

The spatial distribution of events is also a strong observable for background rejection. Since LXe is a strong attenuator for γ rays, background interactions from external sources will occur predominantly near the TPC walls and the PMTs. This is in contrast to the $0\nu\beta\beta\phi$ events, which are expected to have a uniform spatial distribution as a consequence of the uniform dispersion of ^{136}Xe within the LXe. In order to utilise this self-shielding feature of LXe in double beta decay searches, one defines a fiducial volume (FV) within the active LXe, where the external γ rays have attenuated sufficiently so that the resulting background rate is low. The procedure to define such a volume will be discussed in detail in Section 3.5.

3.2 Monte Carlo Simulations

Monte Carlo simulations play a vital role in assessing the design features of the LZ detector, understanding the detector response to $0\nu\beta\beta\phi$ signals, estimating the background rejection efficiency and calculating the residual background activities. LZ has extensive software tools developed to achieve large-scale production of Monte Carlo simulations. The simulation framework begins with BACCARAT [97], which utilises GEANT4 [96] to track particles and their interactions. A detailed model of the LZ detector geometry is included within BACCARAT, with each component linked with an event generator to model the distribution of radioactive sources. The particle tracking and interaction identification information from BACCARAT can then be processed following two separate chains:

- Full chain: this allows for a complete simulation of scintillation photons and ionisation electrons. BACCARAT clusters energy deposits and utilises NEST [75] to calculate the expected number of raw photons and electrons from the interaction. From there, the ionised electrons are simulated to drift to the gas phase and produce the secondary scintillation signal. The scintillation photons are further propagated to hit the PMTs. The response of the PMTs and subsequent electronics chains to photon hits are simulated by the Detector Electronics Response (DER), producing the S1 and S2 signals. This chain renders the most realistic simulation, at the cost of being very computationally intensive and slow for large scale production. Therefore, the full chain is generally used for studies where the requirement on accuracy of individual event reconstruction outweighs the need for high statistics.
- Fast chain: this only records energy deposits and their positions. The chain does not include any information on the PMT photon hits. Instead, detector averaged quantities are quoted and the energy deposit information is passed to NEST to generate the expected S1 and S2 signals. Because the signal generation is based on parametric models only, without the need to reconstruct the event or directly track the large number of optical photons, the fast chain is several orders of magnitude faster than the full chain simulation. The speed of this chain comes at the cost of reduced accuracy, and should be used for studies where high statistics is the priority.

For the purpose of projecting the sensitivity of LZ to $0\nu\beta\beta\phi$, the background model needs to be constructed. This process does not rely on information on the level of PMT photon hits. Instead, it requires high statistics for each background source, such that enough events survive background rejection cuts and give energy spectra that capture important features. Therefore, the majority of analysis work discussed in this chapter utilises the fast chain simulation, unless otherwise specified. The detector parameters within the fast chain simulations are tuned to be in agreement with experimentally obtained values at the time of publication of the SR1 result.

3.3 Detector Signal Response

The response of the LZ detector to $0\nu\beta\beta\phi$ events is studied to determine the signal energy spectrum for each Majoron spectral index, in turn determining the radioactive sources that contribute to the background model. This is achieved by interfacing DECAY0 [100], a Fortran program created specifically for Monte Carlo event generation of nuclear decays in double beta decay searches and dark matter detection, with BACCARAT. The BxDecay0 C++ port of the original DECAY0 is used to generate kinematics of the two outgoing electrons from $0\nu\beta\beta\phi$ events. The resulting 3-momentum information of the electrons is then reformatted and passed to the built-in DECAY0 event generator of BACCARAT for subsequent particle tracking.

The kinematics of different double beta decay processes result in different topology between the outgoing electrons [101, 102]. Integrating over the electron energies, the average angular distribution between the electrons of $0\nu\beta\beta\phi$ takes a simple form $d\Gamma/d\cos\theta = (\Gamma/2)(1 + k\cos\theta)$, where Γ is the decay rate and k is the angular correlation factor that depends on the mode of $0\nu\beta\beta\phi$. For example, the $n = 1$ mode has $k = -0.80$, which means the electrons are preferentially emitted back-to-back [102]. This is shown in Figure 3.1 using simulated particle tracks. Other double beta decay processes may have different angular correlation factor (e.g. $k = -0.66$ for $2\nu\beta\beta$), which provides a useful background rejection tool

for certain experiments (e.g. NEMO-3 and the upcoming SuperNEMO) that can distinguish the electron tracks in a $0\nu\beta\beta\phi$ event.

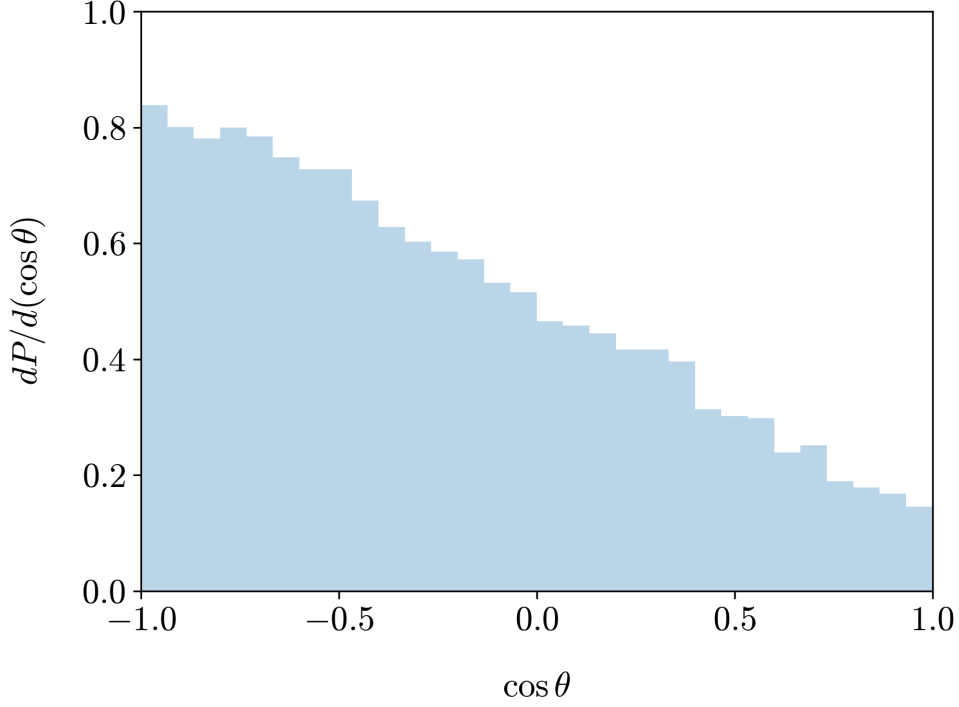


Figure 3.1: Distribution of the angle between the two emitted electrons in $^{136}\text{Xe } 0\nu\beta\beta\phi$.

At the level of $\mathcal{O}(\text{mm})$ electron tracks in LXe, LZ cannot distinguish the $0\nu\beta\beta\phi$ electron topology. As shown in Figure 3.2, almost all of the electron energy deposition sites have a displacement in the z direction, Δz , of less than 2 mm from the decaying nucleus, with the distribution of Δz peaking at about 0.2 mm. Given that the minimal distinguishable vertex separation (scatter resolution) of LZ in the z direction is conservatively estimated to be ~ 4 mm (previous works in LZ have assumed 3 mm [103, 104]), it is evident that the two electron tracks from a $0\nu\beta\beta\phi$ event are not resolved in LZ, resulting in an SS event reconstruction. This indicates that SS events should be considered when searching for $0\nu\beta\beta\phi$ and events that are reconstructed as MS are therefore rejected as backgrounds. Another implication of indistinguishable electron tracks is that an energy-only signal and background model should be assumed throughout the sensitivity projection analysis. The two emitted electrons from a $0\nu\beta\beta\phi$ event are identical in terms of their averaged energy distribution, and

the summed energy distribution follows the energy spectrum of the corresponding spectral index. The single electron and summed electron energy distributions of simulated $n = 1$ events are shown in Figure 3.3.

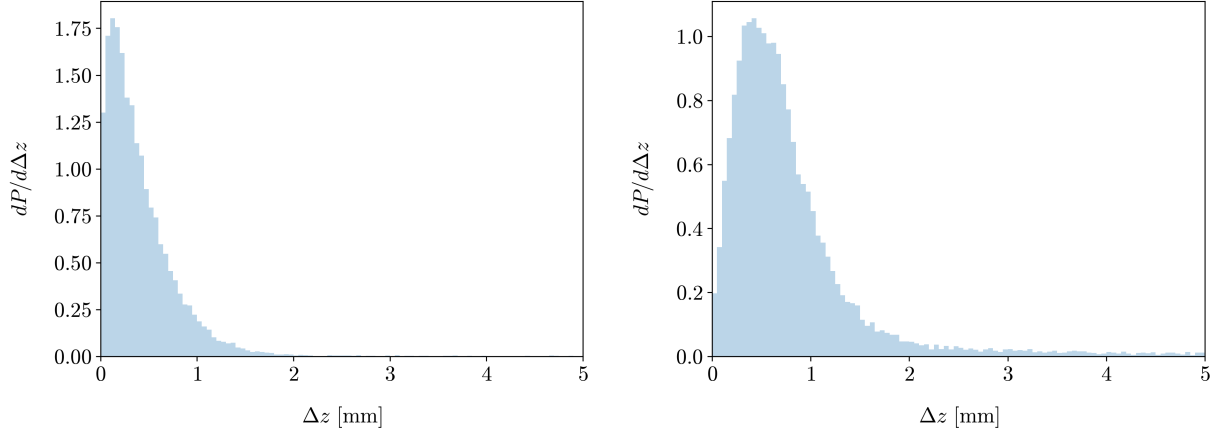


Figure 3.2: Distribution of Δz for simulated electron tracks (left) and all particle tracks (right) in $0\nu\beta\beta\phi$. Electron tracks have Δz below the assumed LZ scatter resolution but a small population of other particles (bremsstrahlung photons) may deposit energy outside this range in the z direction and are therefore reconstructed as multiple scatters.

While all of the primary electron energy deposit sites are in the vicinity of the decaying nucleus with a Δz less than the assumed LZ scatter resolution, the same is not true when considering energy deposits from bremsstrahlung photons. As shown in Figure 3.2, the distribution of Δz for all particles peaks at a slightly higher value at 0.5 mm, with a small fraction of the distribution falling outside the assumed vertical resolution of 4 mm. A population of these events is selected and confirmed the origin of such energy deposits to be bremsstrahlung photons as expected. At the ~ 1000 keV average energy of the individual electrons, the production of bremsstrahlung photons is probable. The emitted photons have a relatively long mean free path. If the photon propagates in a direction away from the x , y plane, its interaction site can have a Δz further than the LZ scatter resolution in the z direction. This leads to events with multiple S2 pulses which are therefore reconstructed as MS by the LZ event reconstruction algorithm. Since the scatter resolution in the horizontal

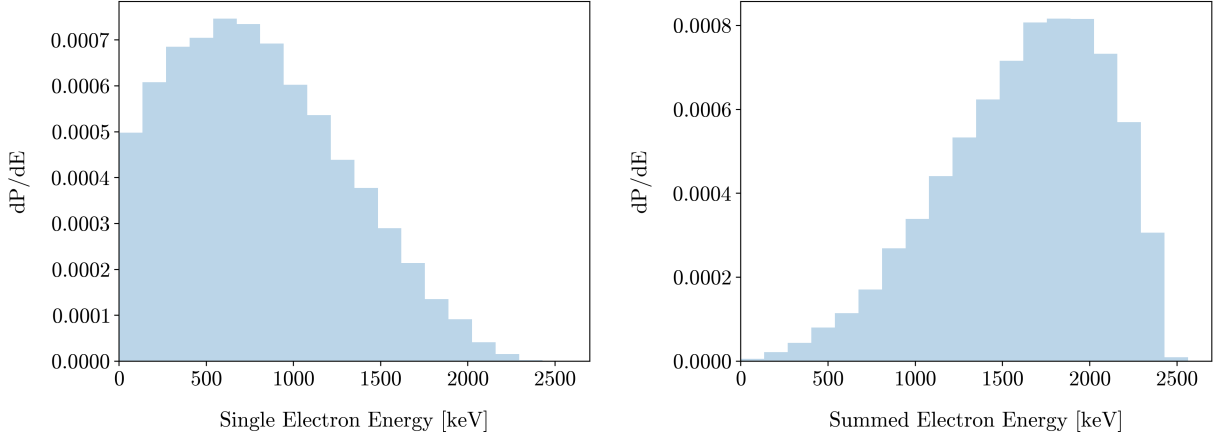


Figure 3.3: Distribution of the energy of a single electron (left) and the summed energy of the two emitted electrons (right) in $^{136}\text{Xe } 0\nu\beta\beta\phi$. The summed electron energy distribution follows the energy spectrum of the corresponding spectral index. Single electron energy distribution is only shown for demonstrative purpose. It is not observable in LZ due to the limitation of scatter resolution, leading to indistinguishable electron tracks in a $0\nu\beta\beta\phi$ event.

plane is of $\mathcal{O}(\text{cm})$, the probability of generating multiple S2 signals will require different algorithms and we conservatively ignore the scatter resolution in the horizontal plane here.

Because the multiplicity of S2 signals is the strongest background rejection tool for $0\nu\beta\beta\phi$ searches, the signal and background models should still be built based on SS events only. In this case, a fraction of $0\nu\beta\beta\phi$ events are excluded due to their MS event reconstruction as a result of the emission of bremsstrahlung photons, leading to a loss in the signal detection efficiency. The cumulative distribution of the maximal Δz in each simulated $0\nu\beta\beta\phi$ event is utilised to quantify the signal detection efficiency. Taking $n = 1$ as an example, 91.3% of the simulated $0\nu\beta\beta\phi$ events have a maximal Δz that is less than the assumed LZ vertical scatter resolution of 4 mm. All of these events should be reconstructed as SS if no further assumption is made on the SS efficiency of the event reconstruction algorithm.

The above signal detection efficiency assumes the full signal energy spectrum as the ROI.

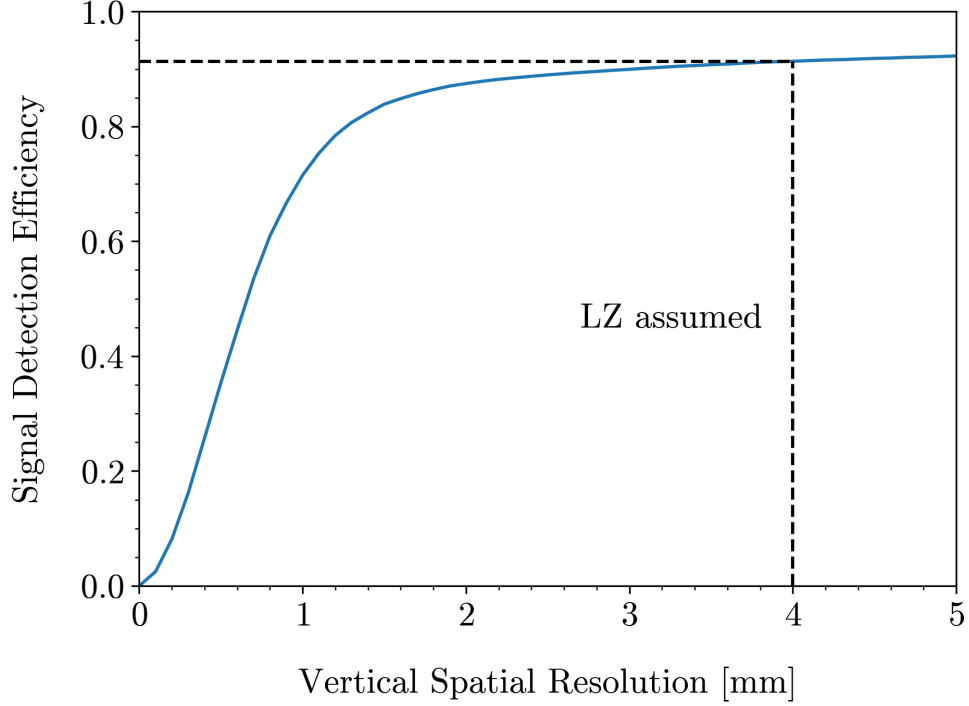


Figure 3.4: Cumulative distribution of Δz as a measure of signal detection efficiency for $n = 1$ $0\nu\beta\beta\phi$ events in ^{136}Xe in LZ.

In practice, due to the optimisation requirements that will be discussed in further detail in Section 3.5, only the ROI section of the energy spectrum is used for signal and background comparison. Since the probability of bremsstrahlung emission increases with energy, the signal detection efficiency should also be energy-dependent. This is in clear contrast to the standard $0\nu\beta\beta$ searches, where the signal is monoenergetic and a single value of signal detection efficiency can be assumed. For $0\nu\beta\beta\phi$ searches, it is more appropriate to define a signal detection efficiency curve, and apply it as a correction to the signal model.

Obtaining the signal detection efficiency curve relies on binning the energy of the simulated $0\nu\beta\beta\phi$ events and calculating the detection efficiency for each bin. Therefore, large statistics are required to ensure an adequate number of events per energy bin for accurate efficiency calculation. It is assumed that the probability of bremsstrahlung emission from electrons at a given energy is independent of the spectral index. Also, the bremsstrahlung emission probability is considered to be negligible at low energies (i.e. 100% of $0\nu\beta\beta\phi$ events are

reconstructed as SS) and increases continuously with energy. With these two assumptions in place, a universal signal detection efficiency curve for all spectral indices can be obtained from the $n = 1$ $0\nu\beta\beta\phi$ simulations alone. The larger fraction of events in the higher energy region can be used to determine the unknown signal detection efficiency in this part of the spectrum.

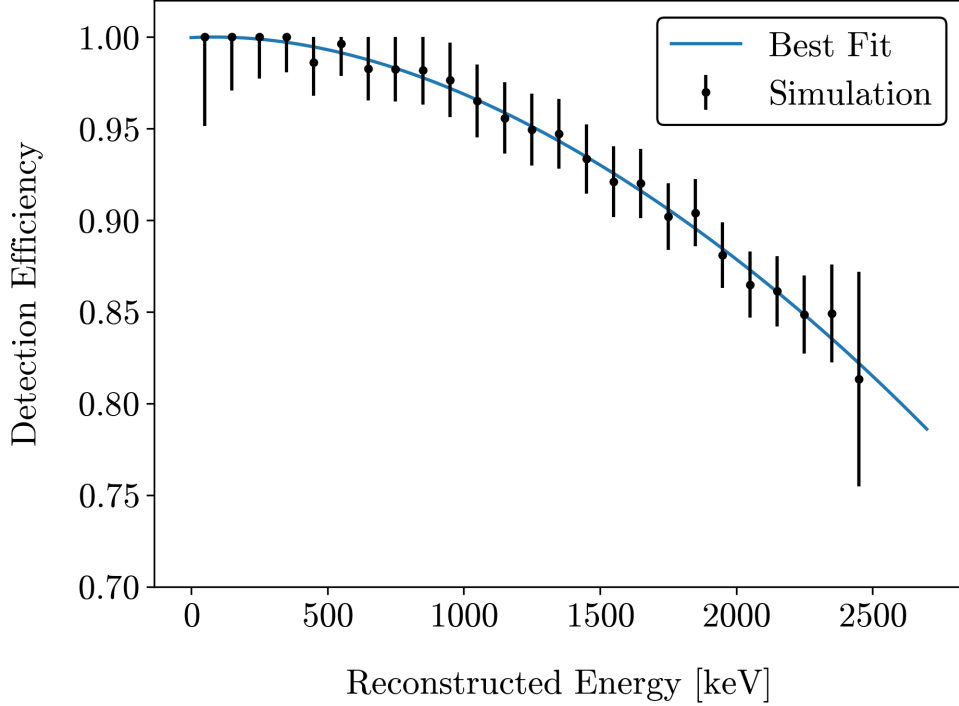


Figure 3.5: Fitting signal detection efficiency correction curve for $0\nu\beta\beta\phi$ in LZ. Asymmetric error bars are used for lower reconstructed energies to reflect the upper bound of 1 for detection efficiency. The curve is extrapolated to 2700 keV to cover the full energy range required for the background model.

The obtained signal detection efficiency curve for $0\nu\beta\beta\phi$ is shown in Figure 3.5. Each data point is the detection efficiency plotted at the centre of the corresponding bin. For the low energy side of the energy spectrum where the bins contains very few or no events, a 100% detection efficiency is assumed given the negligible probability of bremsstrahlung emission. A polynomial fit is then applied to obtain the continuous signal detection efficiency curve. The efficiency is the lowest at about 80% close to the Q-value of the decay.

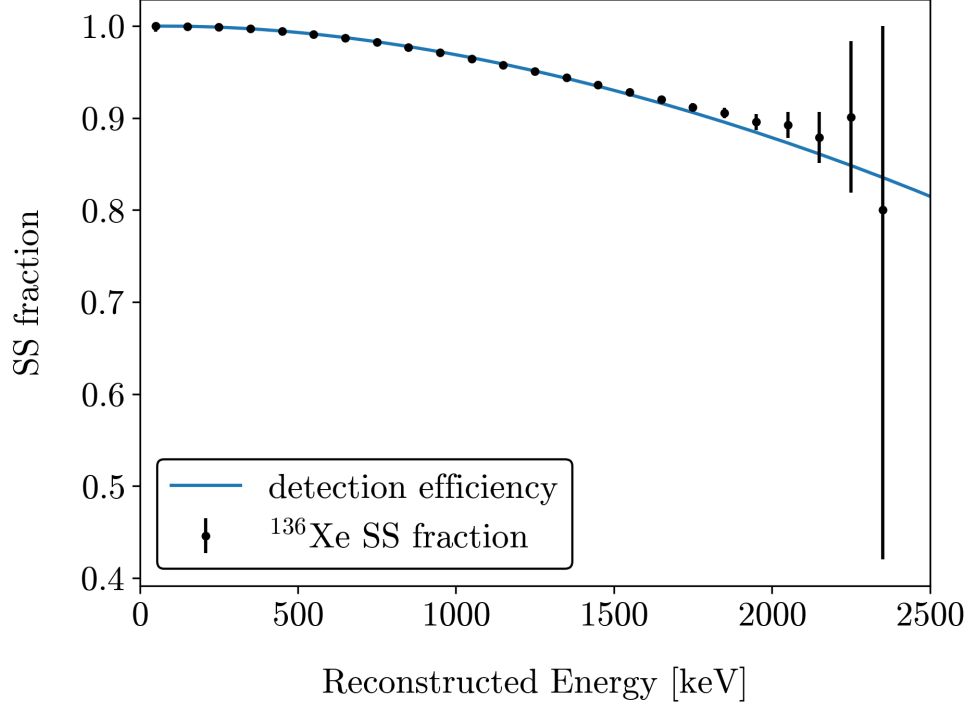


Figure 3.6: Comparison between signal efficiency correction curve and the fraction of SS events in ^{136}Xe $2\nu\beta\beta$ simulation. Asymmetric error bars are used to reflect the upper bound of 1 for the fraction of SS events. The error bars are invisible for lower reconstructed energies due to high statistics of simulated ^{136}Xe $2\nu\beta\beta$ events. The detection efficiency curve agrees well with the ^{136}Xe $2\nu\beta\beta$ simulation up to ~ 2000 keV, above which the low statistics in the energy bins become a limiting factor.

Since the $2\nu\beta\beta$ energy spectrum is equivalent to a $0\nu\beta\beta\phi$ mode with $n = 5$, the exact same detection efficiency curve should apply. The reason not to use $2\nu\beta\beta$ simulations to obtain the curve in the first place is the diminishing statistics at higher energies close to the $Q_{\beta\beta}$ value. Nevertheless, the validity of the signal detection efficiency curve can be cross-checked by the ^{136}Xe $2\nu\beta\beta$ simulations up to ~ 2000 keV, above which the low statistics in the energy bins become a limiting factor. Figure 3.6 demonstrates good agreement between the fraction of events that are classified as SS within the simulated ^{136}Xe $2\nu\beta\beta$, and the $0\nu\beta\beta\phi$ detection efficiency curve. For the remainder of the analysis, unless otherwise specified, this correction curve is applied as a universal correction to $0\nu\beta\beta\phi$ signal energy spectra of all spectral indices.

3.4 Background Sources

Knowing that the $0\nu\beta\beta\phi$ signal events are predominantly reconstructed as SS with no unique event topology for tagging in LZ, the radioactive sources that contribute to the backgrounds in the search for $0\nu\beta\beta\phi$ can be considered in more detail. This section lists these sources, discusses their origin and, where applicable, the background rejection techniques for each one. For the purpose of estimating the half-life sensitivity of LZ over its planned run-time, only radioactive sources that are either long-lived or remained in equilibrium with a stable activity are included. This neglects short-lived radioactive sources such as cosmogenic activation of xenon, which are expected to contribute significantly to the overall activity in SR1 but have since decayed away. We will also consider that neutron activation of xenon isotopes and detector materials during calibration can be neglected, only radioactive sources with broad energy spectra are included due to the spectral shape of $0\nu\beta\beta\phi$ signals.

The origin of the background sources can be classified as either internal or external to the active LXe detection medium. The internal sources are assumed to be uniformly dispersed in LXe and the activity is homogeneous throughout the active volume. One should note that this is a questionable assumption for activation produced during neutron calibrations, which are localised, but this is a sub-dominant contribution. On the other hand, the self-shielding property of LXe leads to strong attenuation of radiation as it propagates towards the centre of the TPC. The difference in spatial distribution of internal and external backgrounds forms the foundation of the FV cut optimisation that will be discussed in Section 3.5. In addition, γ rays from external background sources (detector components and cavern walls) can deposit energy within the Skin or OD region as well as the TPC. Such coincident energy deposition allows the Skin and OD to act as background vetoes that are effective against external backgrounds.

The fast chain simulation is used to generate the energy spectrum for each background source and rescaled to units of events/kg/day/keV. For the purpose of this section, a very minimal set of selection criteria is applied to the simulated data:

- **Single Scatter:** Only events that are classified as SS by the event reconstruction algorithm are selected. This requirement on the multiplicity of S2 signals provides the strongest background rejection on multiple scatter events from external γ rays. It comes at a cost of $< 20\%$ reduction on signal detection efficiency, depending on the energy. For the fast chain simulations, this selection criterion rejects events that have separate NEST clusters with energy-weighted standard deviations (σ_z and σ_r) to be larger than the expected scatter resolutions of the LZ detector [105].
- **Fiducial Volume:** A fiducial volume cut is defined to only keep events with reconstructed position coordinates that are at least 4 cm from the TPC walls, 2 cm above the cathode grid, and 13 cm below the gate grid (i.e. $r < 68.8$ cm, $2 \text{ cm} < z < 132.6$ cm). This choice is made to reject events that may suffer from poor event reconstruction for reasons such as non-uniform electric field line. The LXe mass within the fiducial volume is 5,613 kg, roughly 80% of the active LXe mass in the TPC.
- **Skin and OD Veto:** Backgrounds from γ rays and neutrons can induce coincident activity in the TPC and Skin or OD. The vetoes in this analysis takes the same configuration as those in the LZ SR1 WIMP search [53]. A prompt veto is defined to remove events with OD (Skin) signal within $\pm 0.3 \mu\text{s}$ ($\pm 0.5 \mu\text{s}$) of the TPC S1 pulse. A delayed veto that removes events with large Skin or OD pulses within 1200 μs after the TPC S1 pulse is also applied. This is primarily for thermalised neutrons that are captured on hydrogen or gadolinium in the OD, but also tags γ rays returning to xenon from an OD capture. The long window of the delayed veto is a conservative choice and comes at a cost of 5% false veto rate.
- **Energy:** An energy range of 0–2700 keV is selected when considering the background sources. This range goes beyond the $Q_{\beta\beta}$ value of ^{136}Xe and covers the entirety of $0\nu\beta\beta\phi$ energy spectra for all spectral indices.

Gaussian smearing on the binned reconstructed energy histogram is applied to both the signal and background sources. This was performed by assuming the detector energy resolution model as obtained in LUX [106] and a 1% energy resolution at $Q_{\beta\beta}$ at the time of this

work. (Note that LZ has since achieved a much better 0.67% energy resolution with the SR1 data [1].)

3.4.1 Internal Sources

We begin by plotting each internal background source along with the $0\nu\beta\beta\phi$ energy spectra to illustrate their relative importance in the background model.

Xenon-136 $2\nu\beta\beta$

^{136}Xe in LXe serves as both the signal and a major background source for $0\nu\beta\beta\phi$ searches. The $2\nu\beta\beta$ decay of ^{136}Xe to ^{136}Ba is a Standard Model process. Two electrons and two anti-neutrinos are emitted in the process (along with a residual nucleus), carrying a total energy of $Q_{\beta\beta}$. The observable energy of this decay process comes essentially from the two emitted electrons, while the two neutrinos escape the detector with no energy deposition in the active medium of LZ. The energy spectrum of $2\nu\beta\beta\phi$ is analogous to a $0\nu\beta\beta\phi$ mode with a unique spectral index $n = 5$ that is not shared with any other $0\nu\beta\beta\phi$ decay mode.

^{136}Xe $2\nu\beta\beta$ has a measured half-life of $2.165 \pm 0.016(\text{stat.}) \pm 0.059(\text{sys.}) \times 10^{21}$ years [3]. Assuming a natural abundance of 8.86 ± 0.07 % [107], this is equivalent to $4.14 \mu\text{Bq/kg}$ within the active LXe. It is estimated that the uncertainty in the rate of ^{136}Xe $2\nu\beta\beta$ is 3%, characterised by the spatial uncertainty of the FV cut. As will be discussed in Section 3.5, ^{136}Xe is the most prominent internal background source in the optimal FV and ROI cut for the $0\nu\beta\beta\phi$ search. Therefore, the overall background model is very sensitive to the abundance of ^{136}Xe in the LZ LXe. Figure 3.7 shows that this decay has a continuous energy spectrum that is right skewed, contributing more significantly to backgrounds for a large spectral index such as $n = 7$.

Krypton-85

Natural xenon contains trace amounts of ^{85}Kr , which is a broad spectrum beta emitter. The isotope is uniformly dispersed in the LXe and interacts via ER. LZ conducted a major

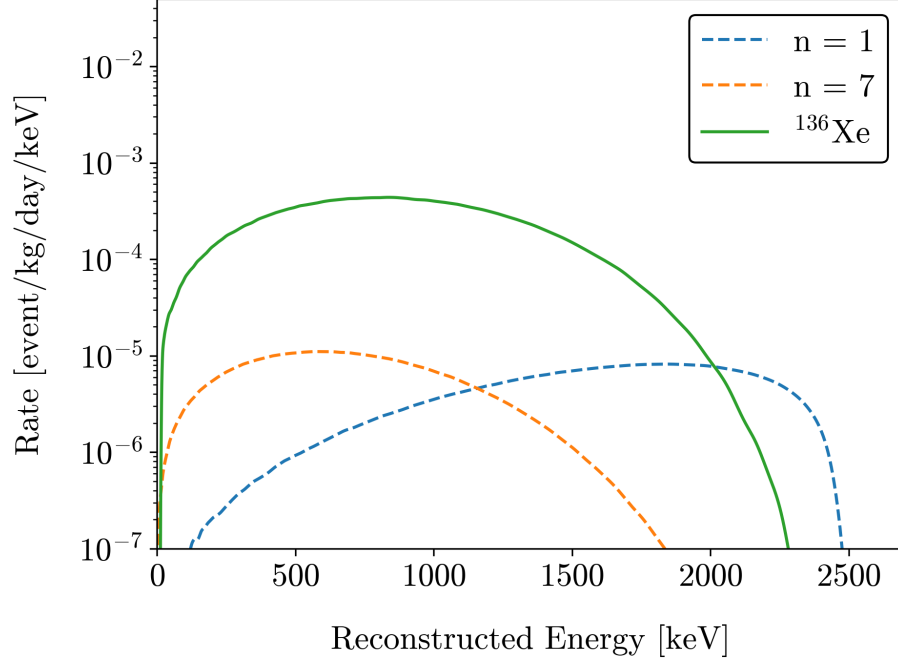


Figure 3.7: Energy spectrum of background events from $2\nu\beta\beta$ in ^{136}Xe . The dotted lines indicate the spectral shape of $n = 1$ and $n = 7$ Majoron-emitting modes scaled arbitrarily for easy comparison.

Kr-removal effort via gas chromatography prior to deployment at SURF [108] to reduce the concentration of krypton to below 1 ppb, in turn lowering the level of ^{85}Kr (typical atmospheric ratio $\sim 2^{-11}$ ($^{85}\text{Kr} / \text{natKr}$) [109]). The concentration of Kr has since been sampled and measured with a highly-sensitive mass spectroscopy technique assisted by a liquid nitrogen cold trap [110] and was continuously monitored during SR1. The frequent monitoring is due to the concern of ^{nat}Kr ingress rate through outgassing of plastics or any leaks in the gas system, which were shown to be negligible during SR1.

The lab measurements and subsequent monitoring show consistent results, leading to a ^{85}Kr rate of 42.3 nBq/kg in the TPC. This is about two orders of magnitude lower than the ^{222}Rn contamination, making ^{85}Kr subdominant in the overall rate of internal backgrounds. The energy spectrum of ^{85}Kr is also shown in Figure 3.8. The spectrum has a Q-value of 687 keV and is therefore most relevant to the $n = 7$ Majoron mode.

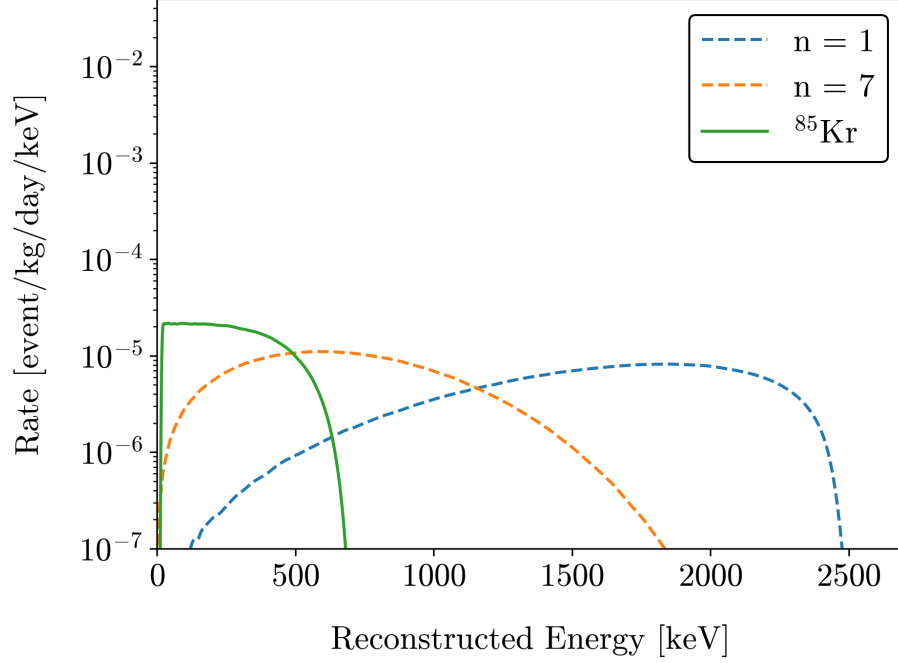


Figure 3.8: Energy spectrum of background events from ^{85}Kr . The dotted lines indicate the spectral shape of $n = 1$ and $n = 7$ Majoron-emitting modes scaled arbitrarily for easy comparison.

Radon Progeny

Radon is naturally produced from decays of thorium and uranium that are present in the detector materials and any dust particles. If in contact with the detector components, radon gas can emanate into the LXe. The radon isotopes are assumed to be uniformly dispersed in the LXe for the purpose of sensitivity projection, though this assumption will be further tested in later chapters. Some β^- -decays of radon and its progeny in subsequent steps along the decay chain can be reconstructed as SS events and contribute to backgrounds of $0\nu\beta\beta\phi$ searches.

There are two radon isotopes of interest: ^{222}Rn and ^{220}Rn . The progeny along the ^{222}Rn decay chain that causes concern for $0\nu\beta\beta\phi$ searches is ^{214}Pb , which undergoes β^- -decay to produce ^{214}Bi . The decay predominantly results in an excited nuclear state of ^{214}Bi , followed by an accompanying γ ray emission from nuclear de-excitation. This typically results in

events being reconstructed as MS and are therefore rejected. However, about 11.0% of the ^{214}Pb beta decay ends in the ground state of ^{214}Bi [111]. These so-called “naked betas” do not have accompanying γ ray emission and are therefore reconstructed as SS. Similarly, the ^{212}Pb progeny along the ^{220}Rn decay chain also undergoes beta decay to produce ^{212}Bi . This process has an 11.9% branching ratio to produce ^{212}Bi in the ground state, leading also to SS event classification.

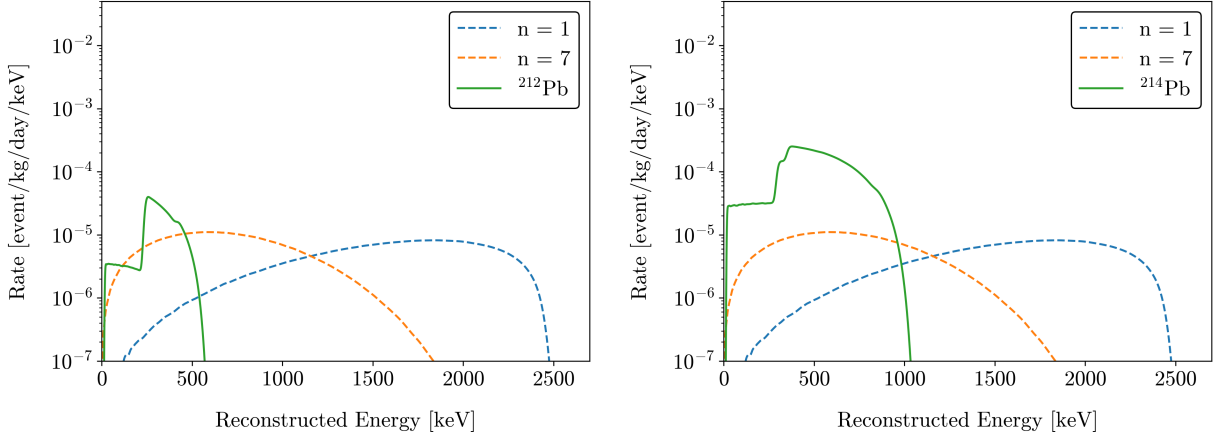


Figure 3.9: Energy spectrum of background events from ^{212}Pb (left) and ^{214}Pb (right). The dotted lines indicate the spectral shape of $n = 1$ and $n = 7$ Majoron-emitting modes scaled arbitrarily for easy comparison.

A contamination level of $1.8 \mu\text{Bq/kg}$ for ^{222}Rn and $0.09 \mu\text{Bq/kg}$ for ^{220}Rn was assumed in the previous LZ WIMP sensitivity study [105], though results from the SR1 dataset suggests higher levels of radon contamination [2]. The ^{214}Pb isotope of concern has a fitted contamination level of $3.26 \pm 0.09 \mu\text{Bq/kg}$ and ^{212}Pb is at $0.137 \pm 0.019 \mu\text{Bq/kg}$. As explained in the LZ SR1 result, the excess radon progeny activity comes from the titanium cryostat and the mechanism of emanation into the TPC requires further investigation. In addition, some of the Rn daughters may be charged ions and drift to the cathode. The effect of this is preliminarily addressed in Chapter 4. A novel ^{214}Pb veto algorithm using liquid flow patterns is under development within the collaboration and preliminary results indicate a $> 50\%$ reduction efficiency. The same algorithm also has the potential to be applied to ^{212}Pb

reduction. This leads to a ^{214}Pb and ^{212}Pb activity in the cleaned data that is well within the previous assumptions. Therefore, for the purpose of background model building and sensitivity projection, a choice is made to reference the same radon contamination levels as in the previous LZ sensitivity studies.

In both the Rn decay chains, the decay steps preceding the Pb isotopes are all alpha decays, with total energy deposition of >5 MeV. Therefore, only the fast chain simulations that start with ^{214}Pb or ^{212}Pb are used. The simulation also includes other beta emitters in the progeny of Pb that can lead to events with SS classification. The overall energy spectra for events in the simulation that pass the selection criteria are shown in Figure 3.9. The rate of ^{214}Pb decays becomes negligible above ~ 1000 keV and the same is true for ^{212}Pb decays above ~ 500 keV. Therefore, backgrounds from radon progeny mostly affect the search for $n = 7$ $0\nu\beta\beta\phi$ mode, where the signal energy spectrum is positively skewed.

Solar Neutrinos

Solar neutrinos undergo electroweak interactions with xenon and induce ER events. The rate is dominated by neutrinos produced in the pp chain, followed by small contributions from ^7Be and the CNO cycle. These contributions are taken into consideration when selecting events from the simulation and building the background model. There are also additional sources of neutrino-induced interactions, including those from coherent elastic neutrino-nucleus scattering (CE ν NS) of ^8B neutrinos, as well as trace amounts from *hep* solar and atmospheric neutrinos. These events have energies less than a few keV and are therefore excluded from the background model.

The aggregated energy spectrum of simulated events from pp chain, ^7Be and CNO cycle neutrinos is shown in Figure 3.10. The spectrum is heavily dominated by low energy ER events and is therefore most relevant to the $n = 7$ Majoron-emitting mode.

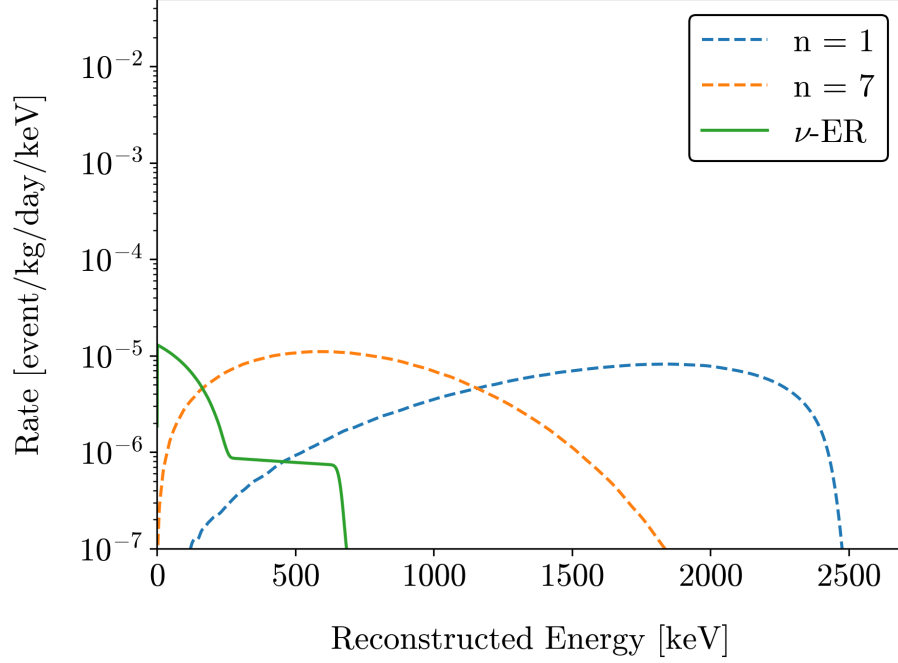


Figure 3.10: Energy spectrum of background events from solar neutrinos. The dotted lines indicate the spectral shape of $n = 1$ and $n = 7$ Majoron-emitting modes scaled arbitrarily for easy comparison.

3.4.2 External Sources

Detector Components

The detector components of LZ contain trace radioisotope contamination and makes up the most prominent contribution to the overall background rate from external sources. Since the radioisotopes are naturally occurring in the materials used to construct the detector components, the contamination is unavoidable. Significant effort has been made to mitigate their effect by searching for the right materials and developing products (e.g. PMTs) with them. This requires a cleaning procedure to be put in place during construction and a comprehensive radioassay campaign [61]. The important radioisotopes to be considered are ^{238}U chain, ^{232}Th chain, ^{60}Co and ^{40}K .

Cobalt-60 is a beta emitter that decays into ^{60}Ni with 99.88% branching ratio into the third excited state [112]. This is predominantly followed by the emission of two subsequent γ rays

of energy 1,173 keV and 1,332 keV, respectively. With the conservatively assumed $Q_{\beta\beta}$ value resolution of 1%, LZ is capable of distinguishing between the two gamma lines, leading to two readily identifiable peaks in the energy spectrum that can be used for both calibration of energy reconstruction and fitting of the background rates. ^{60}Co is present in most of the components constructed from stainless steel (e.g. electrode support rings) and from Kovar (in the PMTs).

Potassium-40 is another naturally occurring radioisotope in detector materials. It primarily decays via beta emission to the ^{40}Ca ground state with branching ratio of 89.25%, forming a continuous energy spectrum. However, it also has 10.55% probability of decaying to the first excited state of ^{40}Ar via electron capture, which is followed by an accompanying γ emission of energy 1461 keV. This γ peak can be utilised for calibration or fitting. An important source of ^{40}K is the potassium used to activate the photosensitive surfaces of all PMTs.

Both the uranium-238 and thorium-232 chains have progeny that undergoes α or β decay. The β decays usually produce excited nuclear states of the decay product and are accompanied by subsequent γ ray emission from nuclear de-excitation. The decays have energies of $\mathcal{O}(\text{keV--MeV})$ which overlaps with the $0\nu\beta\beta\phi$ signal energy range and leads to backgrounds if reconstructed as SS. The ^{208}Tl progeny of the ^{232}Th chain has a notable 2,614 keV γ line that is commonly used for calibration and energy resolution studies. For the ^{238}U chain, its ^{214}Bi progeny produces a number of γ rays with energies greater than 1 MeV and can be used for calibrations and activity fitting. The most prominent one is the 1.76 MeV gamma line with 15.4% relative intensity. Natural uranium also contains 0.3% of ^{235}U but is not included in the background model given its small isotopic abundance.

The energy spectra of simulated events from detector components that survive the selection criteria are shown in Figure 3.11. The simulations for each detector component are sampled based on the results from the LZ radioassay campaign [68] and then assembled for each of the radioisotopes listed. The ^{238}U chain is split into “early” and “late” parts at the level of ^{226}Ra . This is because the 1600-year half-life of the ^{226}Ra interrupts the secular equilibrium

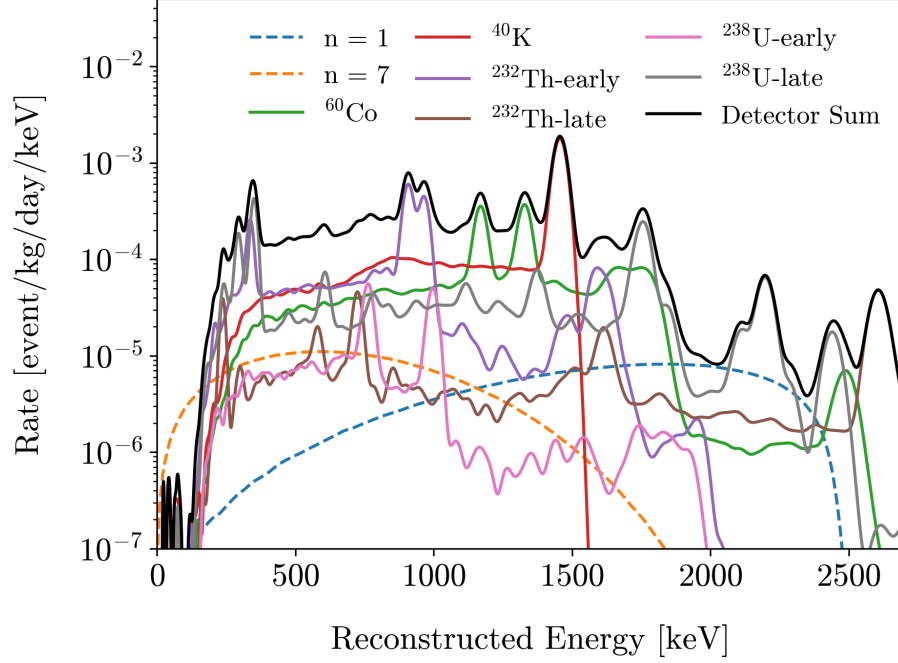


Figure 3.11: Energy spectrum of background events from detector components. The dotted lines indicate the spectral shape of $n = 1$ and $n = 7$ Majoron-emitting modes scaled arbitrarily for easy comparison.

in the chain. Similarly, the ^{232}Th chain is also split into early and late chains, separated by ^{224}Ra . The summed energy spectrum from detector components has considerable rates that span the entire energy range under consideration for the $0\nu\beta\beta\phi$ searches. Therefore, a thorough understanding of the backgrounds from the detector components is essential for Majoron-emitting modes of all spectral indices.

Cavern Rock

The LZ detector is hosted in the Davis Cavern at SURF. The surrounding rock of the cavern has a natural ^{40}K , ^{232}Th and ^{238}U content, with measured activities of 220 Bq/kg, 29.0 Bq/kg and 12.5 Bq/kg, respectively [113]. As discussed above, these isotopes undergo a wide range of decays. Almost all α and β decays from the external cavern are completely contained within the rock itself. The water tank provides significant shielding against external γ rays from the cavern, but the large flux of γ rays still results in some cavern γ events in the active

volume within the TPC, which may be reconstructed as SS events. The OD (and partially the Skin) can be used to actively veto some of the cavern gamma events and mitigate the background rate. The Skin and OD veto cuts applied for event selection are tuned based on the SR1 detector conditions.

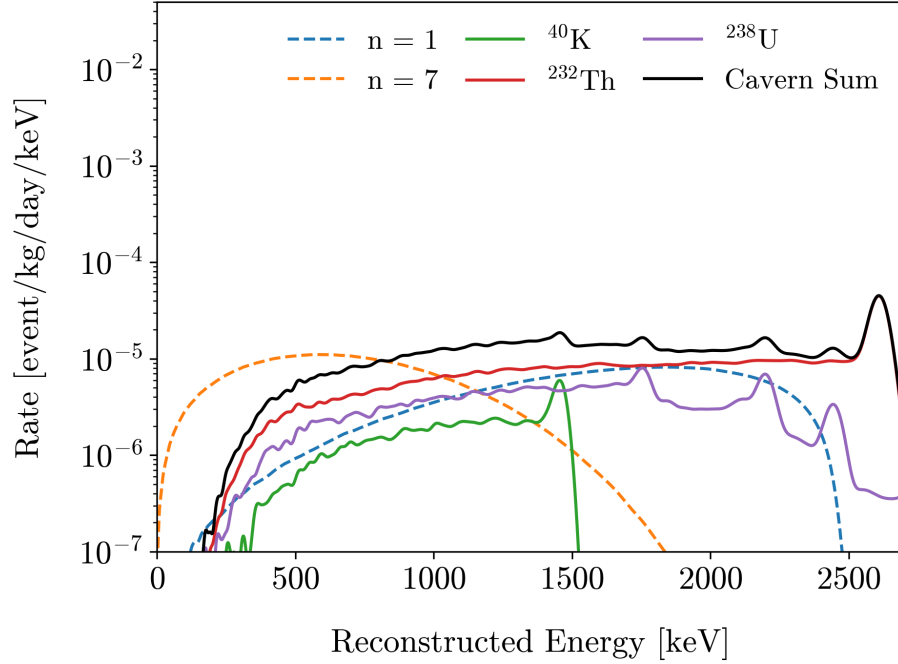


Figure 3.12: Energy spectrum of background events from cavern rock. The dotted lines indicate the spectral shape of $n = 1$ and $n = 7$ Majoron-emitting modes scaled arbitrarily for easy comparison.

The energy spectra of cavern γ events that survive the selection criteria are shown in Figure 3.12. All three spectra follow the same general shape, with peaks at the notable γ lines as stated previously, but diminishes quickly at lower energies due to attenuation. Because the cavern γ backgrounds all have the energy spectra that peak at the high energy γ lines, the background is the most relevant for $n = 1$ $0\nu\beta\beta\phi$ modes, given the negative skewness of the signal spectrum.

3.5 FV and ROI Optimisation

The self-shielding property of LXe strongly attenuates the background rate from external γ rays as one approaches the centre of the TPC. It is common practice to develop a fiducial volume (FV) cut that selects a region in the active LXe volume with relatively low background rate. Because of the symmetry of the detector, the optimal FV is assumed to be a cylinder that can be characterised by its radius and z position coordinates of the top and bottom boundaries. Meanwhile, a region of interest (ROI) energy window should be defined for which the signal and background energy spectra can be compared. Since the $0\nu\beta\beta\phi$ signals are all broad-spectrum, there does not exist a definitive reference energy line (e.g. $Q_{\beta\beta}$ for $0\nu\beta\beta$) for which a narrow energy region can be defined. Therefore, both the FV and ROI are subject to optimisation based on the background model.

The fundamental optimisation strategy is to select FV and ROI cuts that maximise the ratio of signal rate to square-root of the background rate, $S/\sqrt{B}$, based on the concept of signal significance in a counting experiment in the Gaussian regime [114]. The broad-spectrum nature of $0\nu\beta\beta\phi$ signals and backgrounds result in a large $S + B$, typically of $\mathcal{O}(10^3)$ events/day. This ensures that we are in the asymptotic case where the Gaussian approximation holds. The optimisation problem under consideration is the following:

$$\max \quad \frac{S}{\sqrt{B}}(r, z_{min}, z_{max}, E_{min}, E_{max}) , \quad (3.2)$$

where r, z_{min}, z_{max} define the boundaries of a cylindrical FV, and E_{min} and E_{max} define the ROI energy window. Given the difference in the spatial distribution of internal and external backgrounds in LZ and the energy-only search strategy for $0\nu\beta\beta\phi$, an FV cut directly affects the background energy spectrum, which in turn affects the ROI that maximises the $S/\sqrt{B}$. Therefore, the optimisation of FV and ROI are coupled and have to be performed simultaneously.

If carried out by brute force, this multi-parameter optimisation requires significant computational resources to reach ideal granularity. Fortunately, this can be circumvented by carefully designing the optimisation procedure to reduce the computational burden. This

section begins with a discussion on obtaining an estimate for the FV and ROI for each of the spectral indices of $0\nu\beta\beta\phi$. The initial estimates are then used as starting points for the simulated data-driven optimisation procedure. Finally, event selection is applied to simulations to produce the optimised background models for each spectral index. Throughout the FV and ROI optimisation analysis, a Poisson-sampled dataset of simulated background is used to represent an equivalence to 60 days of LZ live time, unless otherwise specified. The dataset has been cleaned to include only events that are reconstructed as SS, as well as passing the Skin and OD veto cuts.

3.5.1 Initial Estimates

The purpose of the initial estimates of ROI and FV parameters is to provide starting points on which a computation-heavy optimisation procedure can be based. For the ROI, this is performed with vetoed background sources for $0\nu\beta\beta\phi$ searches within the same fiducial volume as defined in Section 3.4 ($r < 68.8$ cm, 2 cm $< z < 132.6$ cm). The estimate on ROI relies on identifying the optimal energy window based on spectral shape, rather than the absolute rate. For each spectral index, the $0\nu\beta\beta\phi$ signal energy spectrum is normalised to unity. This is then compared against the energy spectrum of summed internal backgrounds, also normalised to unity, as illustrated in Figure 3.13. The starting energy, E_{min} , and the end energy, E_{max} , are considered in steps of 50 keV and required to be within the 0–2700 keV energy range. A list of possible ROI energy windows are then generated by iterating through all possible combinations of E_{min} and E_{max} . The ratio of area under the signal and background energy spectra is then recorded for each ROI window and the ones that maximises the $S/\sqrt{B}$ are listed in Table. 3.1.

The initial ROI estimates remain fixed and only background rates within these ROI windows are considered for the initial estimates of the FV parameters. In addition, a set of simple assumptions are made when performing the FV estimates:

- The signal and internal background sources are uniformly distributed in the TPC.
- The total background rate within the ROI, B_{total} , is the sum of internal and external

Table 3.1: Summary of initial estimates of ROIs for all major spectral indices.

Spectral Index	$\hat{E}_{min}$ (keV)	$\hat{E}_{max}$ (keV)
$n = 1$	1800	2400
$n = 2$	1500	2350
$n = 3$	650	2200
$n = 7$	0	1300

background rates, B_{int} and B_{ext} .

- For the total volume of the TPC, $B_{ext} > B_{int}$
- Self-shielding eventually creates a central volume where $B_{ext} < B_{int}$

Starting from the relatively quiet central volume, increasing the FV size in both r and z directions increases the signal source exposure in a given live time. Although this inevitably leads to larger B_{int} within the FV, the overall $S/\sqrt{B}$ measure still increases and therefore improves the projected sensitivity. The optimal volume is approximately where $B_{ext} = B_{int}$, as such a volume minimises the external background while maximising exposure to the ^{136}Xe signal source. Further increment of FV will in principle decrease the $S/\sqrt{B}$ measure. The $B_{ext} = B_{int}$ condition enables one to express the optimal radius, $\tilde{r}$, lower boundary, $\tilde{z}_{min}$ and upper boundary, $\tilde{z}_{max}$, in relation to the rate of backgrounds. Following some simple derivations, the optimal parameters of the FV can be estimated by:

$$\begin{aligned} \left. \frac{\partial B_{ext}}{\partial r} \right|_{r=\tilde{r}} &= 6\pi b(z_{max} - z_{min})\tilde{r}, \\ \left. \frac{\partial B_{ext}}{\partial z_{max}} \right|_{z_{max}=\tilde{z}_{max}} &= 3\pi r^2 b, \\ \left. \frac{\partial B_{ext}}{\partial z_{min}} \right|_{z_{min}=\tilde{z}_{min}} &= -3\pi r^2 b, \end{aligned} \tag{3.3}$$

where b is the volume-independent internal background rate, $b = B_{int}/V$. This estimate relies on evaluation of partial derivatives of volume-dependent external background rates

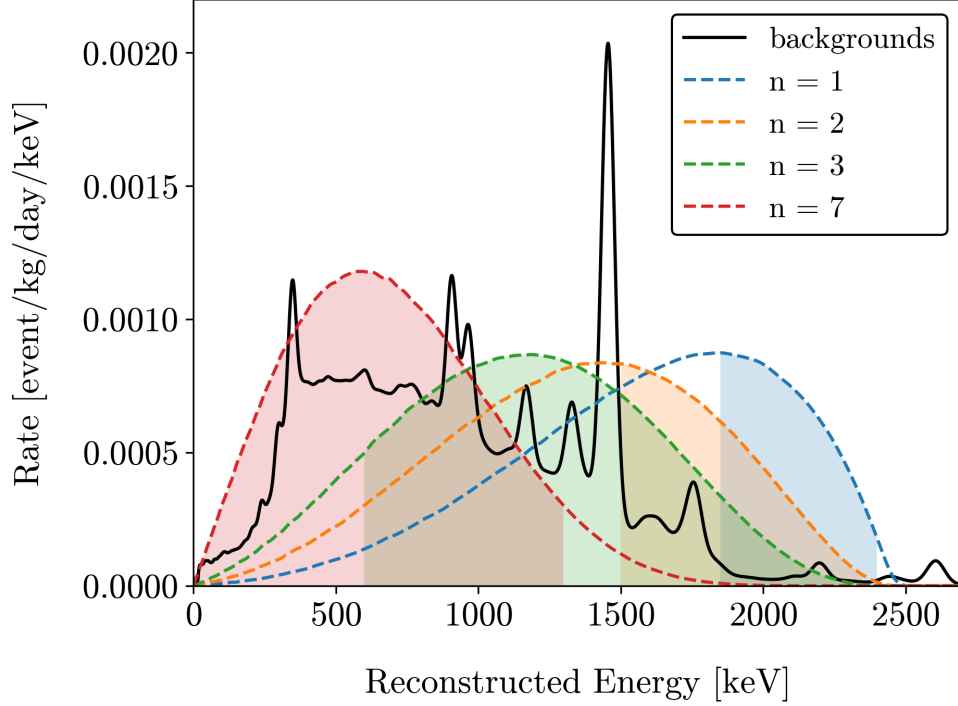


Figure 3.13: Initial estimates of the ROI. The shaded regions indicate the energy windows that have the highest relative $S/\sqrt{B}$ values when comparing against the background energy spectrum.

at specific FV parameters, which cannot be derived analytically. The values are therefore approximated with the Poisson-sampled simulation. An internal cylindrical volume with $r < 39$ cm, $26 \text{ cm} < z < 96$ cm is defined to eliminate the effect of external backgrounds and obtain b . At the estimation stage, only one FV parameter is varied in small steps at a time, while keeping the other two constant, such that the partial derivative of external background rate with respect to the parameter can be approximated. An example of such an estimate for $\tilde{r}$ is shown in Figure 3.14 for the $n = 7$ mode.

The above estimation methodology for optimal FV parameters has been validated against other double beta decay searches within the LZ collaboration. Being another $\beta\beta$ isotope present with significant abundance in natural xenon, ^{134}Xe may also undergo $0\nu\beta\beta$. The process is monoenergetic at $Q_{\beta\beta} = 825.8$ keV [115]. The ROI of this process was set to be $\pm 1\sigma_E$ around $Q_{\beta\beta}$, where σ_E was assumed to be 1.64% at the time. The projected half-life

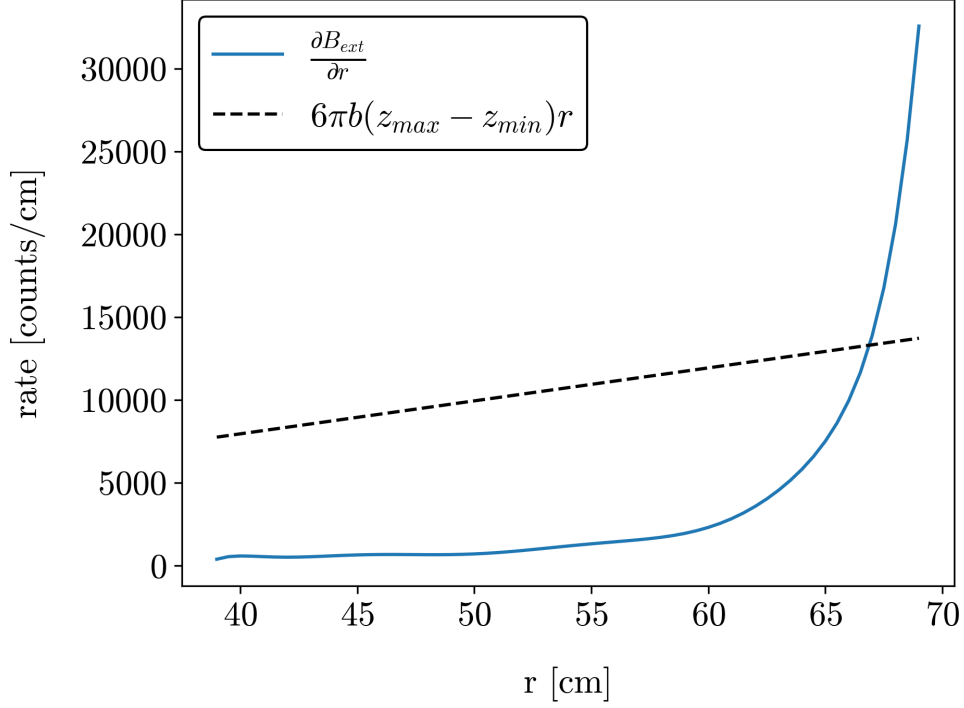


Figure 3.14: Initial estimate of $\tilde{r}$ for the $n = 7$ mode. The optimal value is estimated to be where the solid and the dotted lines intersect

sensitivity of LZ to this process is 7.3×10^{24} years at 90% confidence level (CL) [116]. Utilising an equivalence of 30 live days of Poisson-sampled simulation dataset from the sensitivity study, and the procedure as described above, the optimal FV parameters for $0\nu\beta\beta$ of ^{134}Xe were estimated. These were then compared against the results from a complete scan of FV optimisation presented in the sensitivity study as below:

- Estimate: $\hat{\tilde{r}} = 64$ cm, $\hat{\tilde{z}}_{min} = 4$ cm, $\hat{\tilde{z}}_{max} = 128$ cm
- Scan: $\tilde{r} = 65$ cm, $\tilde{z}_{min} = 10$ cm, $\tilde{z}_{max} = 130$ cm

The $\hat{\tilde{r}}$ ($\hat{\tilde{z}}_{min}$ and $\hat{\tilde{z}}_{max}$) notation indicates the estimate as opposed to the $\tilde{r}$ ($\tilde{z}_{min}$ and $\tilde{z}_{max}$) notation for the scanned optimum. The results showed good agreement for $\tilde{r}$ and $\tilde{z}_{max}$, with only $\tilde{z}_{min}$ not well-predicted, possibly due to the limited statistics in the dataset at the bottom of the TPC. Nevertheless, the agreement is sufficient to support the usage of the estimation method to provide a starting point for later complete optimisation. The resulting estimated

values of optimal FV parameters for each $0\nu\beta\beta\phi$ spectral index are listed in Table. 3.2.

Table 3.2: Summary of initial estimates of optimal FV parameters for all major spectral indices.

Spectral Index	$\hat{r}$ (cm)	$\hat{z}_{min}$ (cm)	$\hat{z}_{max}$ (cm)
$n = 1$	49	23	108
$n = 2$	58	18	121
$n = 3$	64	8	127
$n = 7$	67	5	132

3.5.2 Simultaneous Optimisation and the Background Model

The complete optimisation of FV and ROI need to be carried simultaneously based on the set of parameters ($E_{min}, E_{max}, r, z_{min}, z_{max}$). A brute-force scan of all possible combinations of the parameters is computationally heavy. Starting from the initial estimates of FV and ROI parameters, the following procedure is designed to reduce the computational burden of the problem:

- Fix the ROI at $E_{min} = \hat{E}_{min}$ and $E_{max} = \hat{E}_{max}$
- Start with the estimated $\hat{r}$, $\hat{z}_{min}$ and $\hat{z}_{max}$. Successively relax one parameter (e.g. r) at a time and scan around the initial estimate
- Record the relative $S/\sqrt{B}$ values within the FV and fit a curve to find the optimal parameter (e.g. $\tilde{r}$)
- Replace the fixed parameter from the initial estimate to the optimal (e.g. $\hat{r}$ to $\tilde{r}$) then repeat for the other two FV parameters
- Record the optimal $S/\sqrt{B}$ value and the corresponding $\tilde{r}, \tilde{z}_{min}, \tilde{z}_{max}$
- Change the ROI and repeat the steps

The E_{min} and E_{max} values are varied around their initial estimates and the FV optimisation procedure is performed for each ROI. Only the $S/\sqrt{B}$ value at the optimal set of FV parameters is recorded, which is then compared with the optimal $S/\sqrt{B}$ for other ROIs. Such

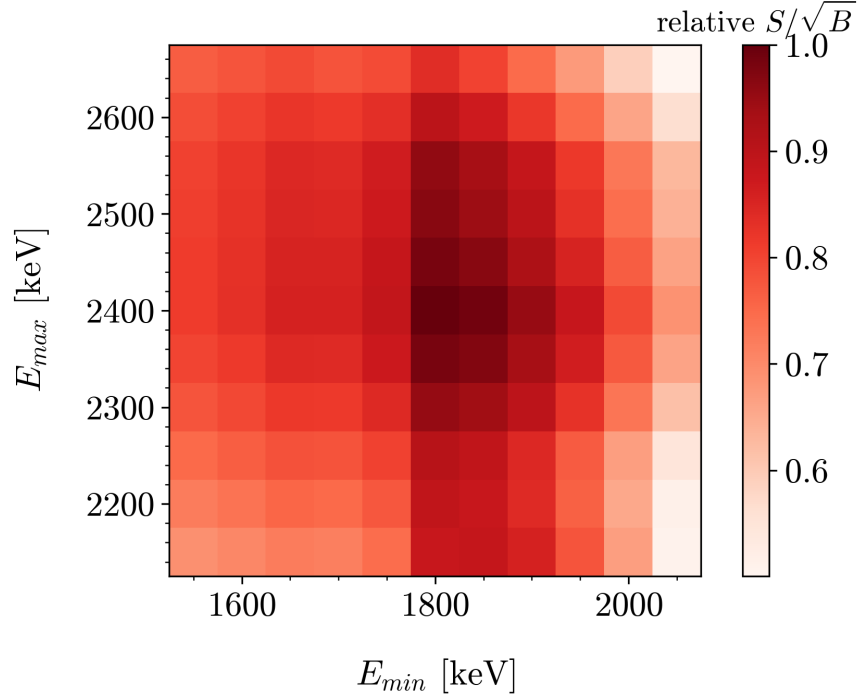


Figure 3.15: The optimal relative $S/\sqrt{B}$ as a function of E_{min} and E_{max} for the $n = 1$ mode.

A global optimal ROI is found to be 1800–2400 keV and deviation from this ROI results in lower relative $S/\sqrt{B}$.

a comparison determines the energy window within which the optimal $S/\sqrt{B}$ is a global maximum, and the corresponding FV parameters are the global optima. An example of such a comparison is shown in Figure 3.15 for $n = 1$ mode, where a maximum is clearly visible. The optimised ROI and FV parameters for each of the spectral index are listed in Table. 3.3, as well as the LXe mass within the optimised FV.

3.6 Sensitivity Projection

The projected sensitivity of LZ to $0\nu\beta\beta\phi$ is defined as the lower limit on the half-life that the experiment cannot exclude, corresponding to the 90% CL upper limit on the number of signal events. The projected sensitivity can be expressed as

$$T_{1/2} \geq \frac{N_{136\text{Xe}}}{N_s^{\text{upper}}} \epsilon_s t \ln 2, \quad (3.4)$$

Table 3.3: Summary of the optimised FV parameters for all major spectral indices.

Spectral Index	$\tilde{E}_{min}$ (keV)	$\tilde{E}_{min}$ (keV)	$\tilde{r}$ (cm)	$\tilde{z}_{min}$ (cm)	$\tilde{z}_{max}$ (cm)	Mass (kg)
$n = 1$	1800	2400	66.7	12.9	125.7	4531
$n = 2$	1500	2350	65.9	14.9	129.6	4497
$n = 3$	700	2300	66.8	10.4	129.9	4814
$n = 7$	0	1300	68.7	6.8	133.4	5394

where $N_{136\text{Xe}}$ is the number of source ^{136}Xe atoms, N_s^{upper} is the 90% CL upper limit on the number of signal events, ϵ_s is the signal efficiency as a result of both the detector response and the ROI over which $0\nu\beta\beta\phi$ is searched, and t is the cumulative live time of the experiment.

The $0\nu\beta\beta\phi$ modes all have continuous electron energy spectra with distinctive spectral shape. While a simple counting experiment can still be performed, a more sophisticated approach is to apply a maximum-likelihood based analysis and boost the projected sensitivity with the spectral shape information. This section introduces the statistical methods to perform such a likelihood-based analysis, then presents the results of sensitivity projections utilising the signal and background model introduced in Section 3.3 and Section 3.5, respectively.

3.6.1 Profile Likelihood Ratio

The key to obtaining a projected sensitivity is to determine the upper limits of signal events under the background-only hypothesis. For LZ, this is achieved with hypothesis testing under the frequentist interpretation of probability. The key to hypothesis testing is to have two sets of hypotheses, a “default hypothesis”, H_0 , and the “alternative hypothesis”, H_1 , based on the physics being studied. A subtle caveat to note is that the term “null hypothesis” is commonly used to refer to H_0 in statistics literature, but in the context of many physics experiments, the term “null hypothesis” generally refers to the background-only case and is not necessarily the default hypothesis under test.

Instead of performing the hypothesis test on the dataset, X , a single-valued test statistic $T(X)$ is used to summarise the dataset and allow statistical statements to be made. The separable distributions of X under the two hypotheses result in distinct distributions of $T(X)$. If the observed dataset, X_{obs} , gives a test statistic that falls in an extreme “critical region” of $T(X)$ with small probability under H_0 , the hypothesis is rejected. Mathematically this means H_0 is rejected in favour of H_1 if

$$P(T \geq T(X)|H_0) \leq \alpha, \quad (3.5)$$

where α is the size of the small probability, or significance level of the test. The confidence level is simply $1 - \alpha$ and can be interpreted as the probability of successfully rejecting the default hypothesis. The conventional choice in this field is to reject the default hypothesis at 90% CL.

In rare event searches, including various double beta decays and dark matter detection, it is common to adopt the profile likelihood ratio (PLR) as the test statistic [117]:

$$\lambda(\mu) = \frac{L(\mu, \hat{\hat{\theta}}(\mu))}{L(\hat{\mu}, \hat{\theta})}. \quad (3.6)$$

Here μ is the expected number of signal events and is our parameter of interest (POI), θ is a vector of the nuisance parameters contained within the signal and background model (e.g. background rate of a particular component) whose values are not known *a priori* and need to be fitted with data, and L is the likelihood. The symbols $\hat{\mu}$ and $\hat{\theta}$ denote the global unconditional maximum-likelihood estimators (MLEs) of the parameters, whereas $\hat{\hat{\theta}}$ denotes the conditional MLEs of the nuisance parameters under the value of μ being tested. It is evident from the definition of $\lambda(\mu)$ that it takes a value in the range $0 \leq \lambda(\mu) \leq 1$. If the value is near 1, the data are considered to be in good agreement with the hypothesised value of μ under test.

The $0\nu\beta\beta\phi$ search in LZ presented in this work is restricted to an energy-only analysis, with the signal and each background source modelled with a probability density function (PDF) $P(E)$. Given a dataset of N events, the PDFs are combined to form an extended likelihood

function

$$L(\mu_s, \{\mu_b\}) = \frac{\mu^N e^{-\mu}}{N!} \prod_{i=1}^N \left[\left(\mu_s P_s(E) + \prod_{j=1}^{n_b} \mu_b^j P_b^j(E) \right) \prod_{k=1}^{n_b} \mathcal{N}(a_b^k, \sigma_b^k) \right]. \quad (3.7)$$

Here μ is the total expected number of events from the signal and background sources combined, $\mu = \mu_s + \sum_{i=1}^N \mu_b$, with μ_s events from the signal source and μ_b^i events from the i -th background source. A set of nuisance parameters are assigned to the expected background rates a_b^k and their systematic uncertainties σ_b^k , all of which are included in the Gaussian constraint terms $\mathcal{N}(a_b^k, \sigma_b^k)$.

For the purpose of sensitivity projection, some modification to the test statistic is necessary. The logarithm of $\lambda(\mu)$ is taken since log likelihoods are additive and mathematically more treatable. In addition, the nature of $0\nu\beta\beta\phi$ search implies that the presence of any physical signal always increases the mean event rate ($\mu \geq 0$). It is therefore conventional to define the following one-side PLR statistic:

$$q_\mu = \begin{cases} -2 \ln \lambda(\mu), & \hat{\mu} < \mu \\ 0, & \hat{\mu} \geq \mu \end{cases}, \quad (3.8)$$

where $\lambda(\mu)$ is the original PLR statistic as defined in Eq. 3.6. This test statistic ranges from 0 to ∞ , with the larger values indicating increasing level of incompatibility between the hypothesised value of μ and the dataset.

Hypothesis testing of q_μ is performed by scanning over a range of values of μ . In each test, the default hypothesis is the presence of μ signal events plus backgrounds (S+B), whereas the alternative hypothesis is taken as background-only (B). The level of compatibility of each hypothesised value of μ with data is measured by calculating the p -value

$$p = \int_{q'_\mu}^{\infty} f(q_\mu | S + B) dq_\mu, \quad (3.9)$$

where q'_μ is the value of the test statistic at the given μ and $f(q_\mu | S + B)$ is the distribution of q_μ under H_0 .

Computation of the p -value requires integrating over the distributions of the test statistic. This can be performed numerically with toy Monte Carlo simulations. The procedure starts with simulating a certain number of events that is drawn from the Poisson distribution with a mean under the S+B hypothesis. The events have simulated values of the observable: in the case of $0\nu\beta\beta\phi$ this is the reconstructed energy E . For each of the simulated experiments, the test statistic q_μ is evaluated for that given value of μ . The test experiments are repeated many times to establish a distribution for q_μ , which then enables calculation of p -values for the hypothesis. This is then repeated for all considered values of μ . Given the broad-spectrum nature of $0\nu\beta\beta\phi$ and the large number of expected signal events, the toy data are binned to reduce computational power required for the analysis.

Provided that suitable regularity conditions are met, one can assume the asymptotic limit where the sampling distribution of both $f(q_\mu|S+B)$ and $f(q_\mu|B)$ can be approximated analytically by Wilks' theorem [117]. The necessary conditions for Wilks' theorem are listed in Ref. [118], all of which are applicable to the $0\nu\beta\beta\phi$ search with a suitable choice of test statistic [117]. For the purpose of sensitivity projection, the asymptotic limit approach is adopted to expedite the analysis.

3.6.2 Projected Sensitivity

The likelihood function Eq. 3.7 requires inputs of the nuisance parameters that define the initial values of the expected background rates a_b^k and the corresponding systematic uncertainties σ_b^k for each background source. Table 3.4 summarises the relative uncertainties of each source in the background model. For detector components, the uncertainties are estimated from simulation and kept in agreement with previous sensitivity projection results from LZ [104, 105, 116]. The ^{136}Xe uncertainty comes from half-life measurement [3] and that of neutrino interactions comes from flux uncertainty [119]. All of the remaining uncertainties are inferred from LZ measurements either during calibration or the SR1 data-taking period, as reported in Ref. [2]. Since the analysis uses an ROI to achieve the optimal sensitivity, certain background sources may have zero expected rate within the ROI despite their significant contribution when considering the full spectrum. For example, the ^{214}Pb

energy spectrum only spans up to about 1000 keV and is expected to have zero contribution to the ROI in the 1800–2400 keV region. In such cases, the sources are removed from the background model.

Table 3.4: Summary of the relative uncertainties on the rates used in the likelihood function for individual background sources. The uncertainties for detector components are estimated from simulation [104, 105, 116], while those for other components come from measurements, either by other experiments in the case of ^{136}Xe [3], or inferred directly from LZ results [2].

Background Location	Source	Relative Uncertainty
Detector components	^{60}Co	30%
	^{40}K	30%
	^{232}Th -early	30%
	^{232}Th -late	30%
	^{238}U -early	30%
	^{238}U -late	30%
Cavern rock	^{40}K	15%
	^{232}Th chain	10%
	^{238}U chain	30%
Internal sources	^{85}Kr	15%
	^{212}Pb	15%
	^{214}Pb	5%
	^{136}Xe	3%
	ν -ER	2%

Figure 3.16 shows an example of the upper-limit setting for the $n = 1$ mode of $0\nu\beta\beta\phi$ with 500 live days by scanning over a range of hypothesised μ_s . The resulting median upper limit at 90% CL is $\mu_{upper} = 759$, which translates into a half-life sensitivity of $T_{1/2} \leq 4.75 \times 10^{23}$ yr at 90% CL through Eq. 3.4. This is within an order of magnitude from the current upper limit of 4.3×10^{24} yr [38] set by EXO-200 with high ^{136}Xe enrichment. The result also has

scope for improvements due to the conservative choices made when considering the energy resolution, the ^{214}Pb and ^{212}Pb veto efficiency, the relative uncertainties, as well as the possibility of LZ fulfilling its goal of 1,000 live days as proposed. Regardless of the possible future improvements, the current conservative projected sensitivity already demonstrates the potential of LZ as a multi-purpose experiment outside its primary science goal of WIMP detection.

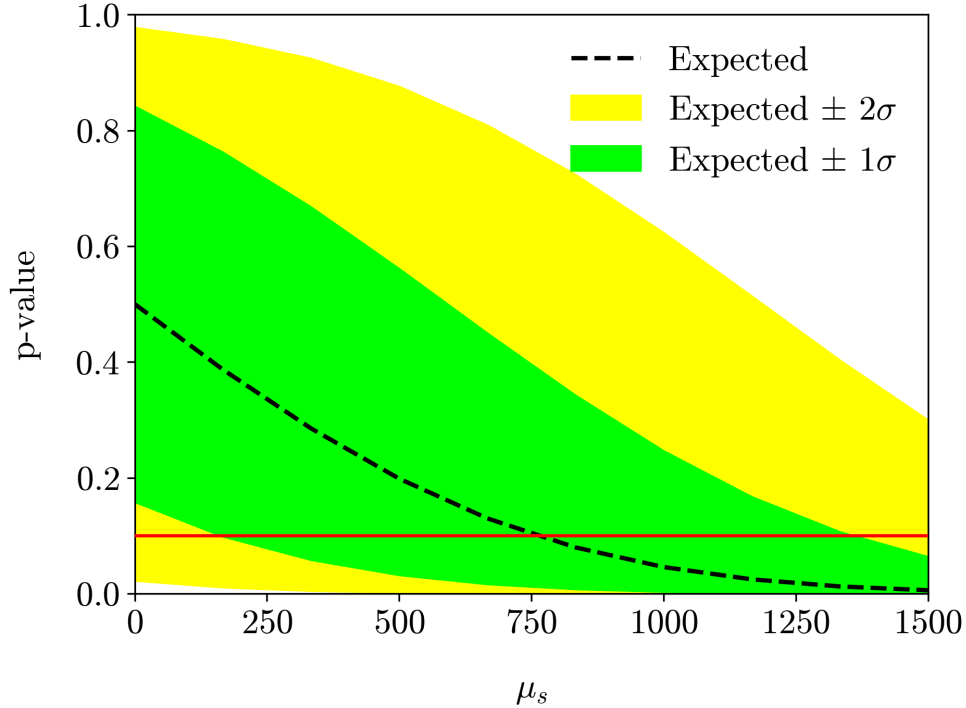


Figure 3.16: p-values of a hypothesised LZ run of 500 livedays to search for the $n = 1$ mode of $0\nu\beta\beta\phi$. The calculation assumes the default hypothesis of signal plus background (H_0) and the alternative hypothesis of background-only (H_1). The dashed line represents the median p-value and its intersection with the solid red line indicates the 90% CL upper limit. The green (yellow) region indicates the $\pm 1\sigma$ ($\pm 2\sigma$) statistical uncertainty.

We can now go beyond the $n = 1$ mode. Figure 3.17 shows the evolution of projected sensitivity with respect to the number of live days for $0\nu\beta\beta\phi$ modes with major spectral indices. Unlike in the $n = 1$ case where dedicated experiments have distinctive advantages, the LZ projected sensitivities become very competitive against current best limits for higher

spectral indices, especially for $n = 7$. The strong performance of LZ for higher spectral indices stems from its optimised backgrounds in the low-energy end of the spectrum (for WIMP detection). Dedicated experiments such as EXO and KamLAND-Zen are usually limited by their energy threshold at ~ 500 keV. With an ER energy threshold that goes below 1 keV [53], LZ is able to capture sensitivity from the skewness of the signal energy spectra. With even a conservative total run-time of 500 live days, LZ has the potential to be one of the most sensitive experiments to some major modes of ^{136}Xe $0\nu\beta\beta\phi$.

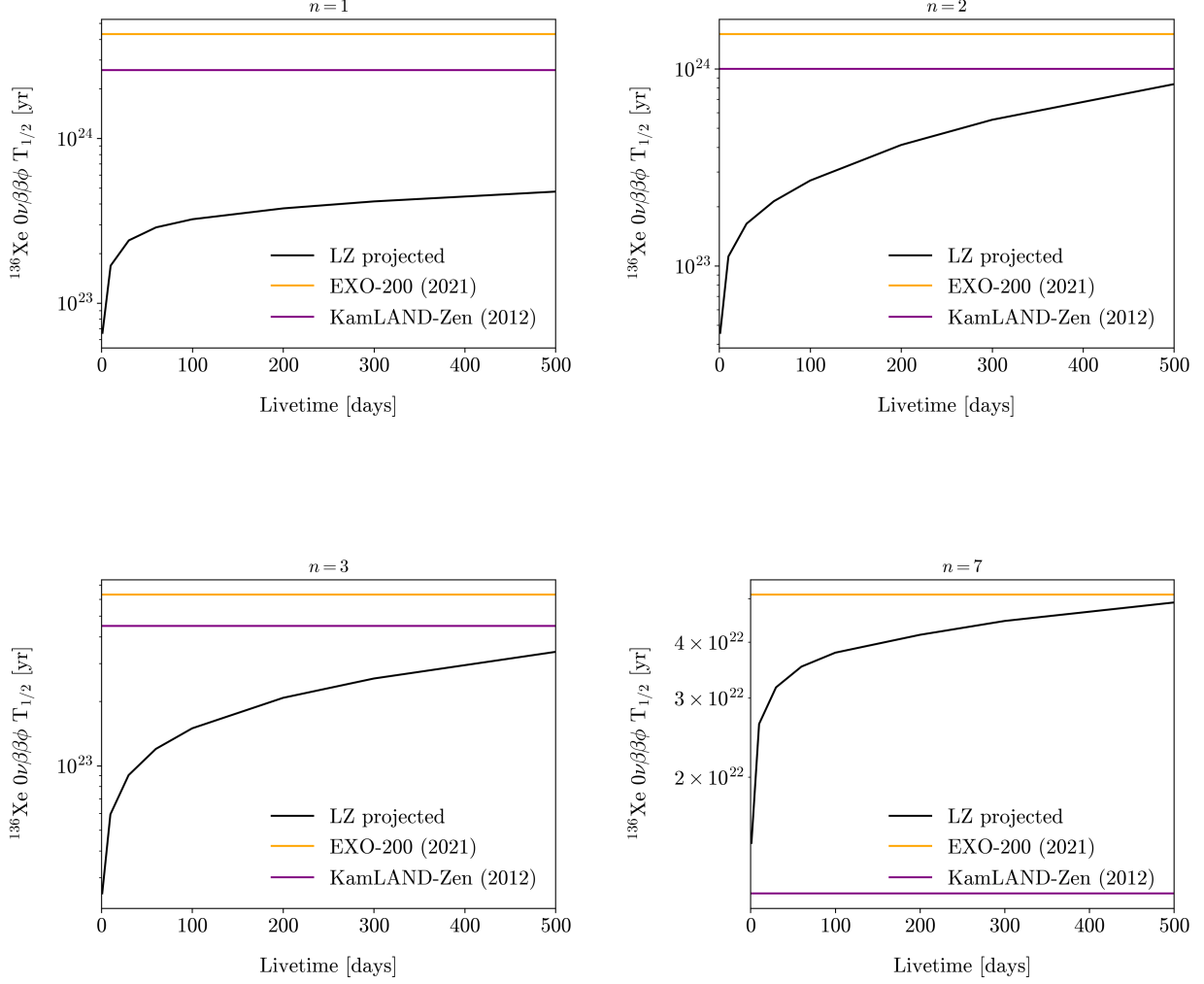


Figure 3.17: LZ projected half-life sensitivity to $^{136}\text{Xe } 0\nu\beta\beta\phi$ decay as a function of detector live time. For comparison, the limits set by EXO-200 [38] (solid orange) and KamLAND-Zen [46] (solid purple) are also shown as horizontal lines that do not vary with the LZ detector live time.

Chapter 4

Radon Non-uniformity and ^{214}Pb Spatial Distribution

This chapter focuses on the impact of radon and its progeny on $0\nu\beta\beta\phi$ searches in LZ. An overview of the radon decay chains and their prominent progeny is provided. This is followed by discussion on the spatial non-uniformity of radon progeny, a phenomenon that has only recently been observed in the multi-tonne scale xenon TPC of LZ. Methods of studying the spatial distribution of ^{214}Pb , the dominant radon progeny relevant for $0\nu\beta\beta\phi$ searches, will be discussed. These include a novel tagging method and a preliminary toy Monte Carlo approach. This chapter concludes with an estimate of the impact of ^{214}Pb spatial distribution on the projected sensitivity of LZ to $0\nu\beta\beta\phi$.

4.1 Radon Decay Chains

Radon is a decay product of uranium and thorium, both of which are naturally present in detector materials and dust particles. As radon gas comes into contact with detector components, it can diffuse into the xenon spaces and disperse throughout the active volume. Radioactive decays of radon and its progeny within the LXe become important background sources. In the context of $0\nu\beta\beta\phi$ searches, the nuclides ^{214}Pb and ^{212}Pb from the radon decay chains are particularly important in the background model, especially in the lower end of the energy spectrum. Previous Monte Carlo simulations have assumed that radon

and its progeny are uniformly dispersed in LXe. However, whether this assumption holds true in real LZ data is subject to further investigation and tests.

There are two radon isotopes that are of particular interest to LZ: ^{222}Rn and ^{220}Rn . They occur as intermediate steps in distinct decay chains. ^{222}Rn has a half-life of 3.82 days and is part of the ^{238}U chain. The expected activity of ^{222}Rn is less than $2.0\ \mu\text{Bq/kg}$ in the active LXe volume in LZ, as specified in the LZ technical design report [61]. On the other hand, ^{220}Rn is a shorter lived isotope with a half-life of 55 seconds. It exists in the ^{232}Th chain and is expected to have a much lower activity in LZ, estimated to be less than $0.2\ \mu\text{Bq/kg}$ in the active LXe. It is important to note that in both decay chains, all decay products preceding radon accumulate within the solid materials containing uranium or thorium and do not enter the active xenon volume. For the purpose of understanding internal background sources in LXe, the focus is on radon isotopes and their progeny. Due to the high ionisation density and recombination probability of α particle tracks, a high-energy α decay event can be easily identified based on its S1 to S2 ratio. Therefore, the main contribution to backgrounds of $0\nu\beta\beta\phi$ searches in radon decay chains come from β emitters.

An overview of the dominant decays (BR>99%) of the ^{222}Rn chain is shown in Figure 4.1. The decay chain starts with two consecutive highly energetic α decays, each releasing about 6 MeV of energy and producing the ^{218}Po and ^{214}Pb progeny. The α particles emitted from ^{222}Rn and ^{218}Po decay events are generally expected to be classified as SS in LZ, with a small fraction of misclassified population for various reasons, such as the absence of S2 signals near the TPC wall due to electron attachment on the PTFE panels.

Following the initial α decays, there is a β emission from ^{214}Pb with a continuous spectrum of energies below its Q-value of 1.02 MeV. The majority of these decays produce excited nuclear states of ^{214}Bi and are accompanied by emission of γ rays. Such events are expected to be classified as MS, provided that the γ rays interact with LXe and deposit energy at a vertical distance greater than the z scatter resolution of the TPC. However, a considerable fraction ($\sim 11.0\%$ [111]) of the β decays end up in the ground state of ^{214}Bi without any

accompanying γ emission. These “naked” β decays are challenging to identify and directly contribute to the backgrounds for $0\nu\beta\beta\phi$ searches.

The subsequent steps in the decay chain are a β emission of ^{214}Bi , followed almost instantly by an α emission from ^{214}Po . The time separation between them is characterised by the short 164 μs half-life of ^{214}Po . The combination of the two decay steps form the signature Bi-Po events in the ^{222}Rn decay chain. In theory, the Bi-Po events should be classified as MS, but their classification can be complicated in practice. If the ^{214}Bi β decay produces an excited nuclear state of ^{214}Po , the accompanying γ ray emission can scatter multiple times and give rise to several S2 signals itself. There are also possibilities of overlapping signals from the β and α decays, reducing the number of S2 signals in the event. The ^{222}Rn decay chain then continues with a series of consecutive β emissions and an energetic α emission. The half-lives of these isotopes are relatively long and their activities are therefore subdominant. The ^{222}Rn chain terminates at the stable ^{206}Pb isotope.

The other relevant decay chain is that of ^{220}Rn . Although it shares similarities with the ^{222}Rn chain, it is expected to have a much lower activity in the active LXe. An overview of the dominant decays of this chain is shown in Figure 4.2. The chain can be divided into the fast and slow components, with ^{212}Pb as a separation point between them due to its longer half-life than other isotopes in the chain. The fast component consists of two high-energy α emissions. Similar to the ^{222}Rn chain, these events are expected to be reconstructed as SS due to the high ionisation density of α particles. The ^{212}Pb which follows the initial α decays is a β source with a 11.9% branching ratio into the ground state of ^{212}Bi [111]. This leads to the production of “naked” β events that do not have associated γ emission, and they are expected to be reconstructed as SS. These events are also backgrounds for $0\nu\beta\beta\phi$ searches, though the lower activity of ^{220}Rn in active LXe makes the ^{212}Pb β decay rate subdominant in comparison to that of ^{214}Pb .

The ^{220}Rn chain then splits into two possible paths, both ending at the stable ^{208}Pb isotope. The first path is the Bi-Po events with a time separation characterised by the ^{212}Po half-life

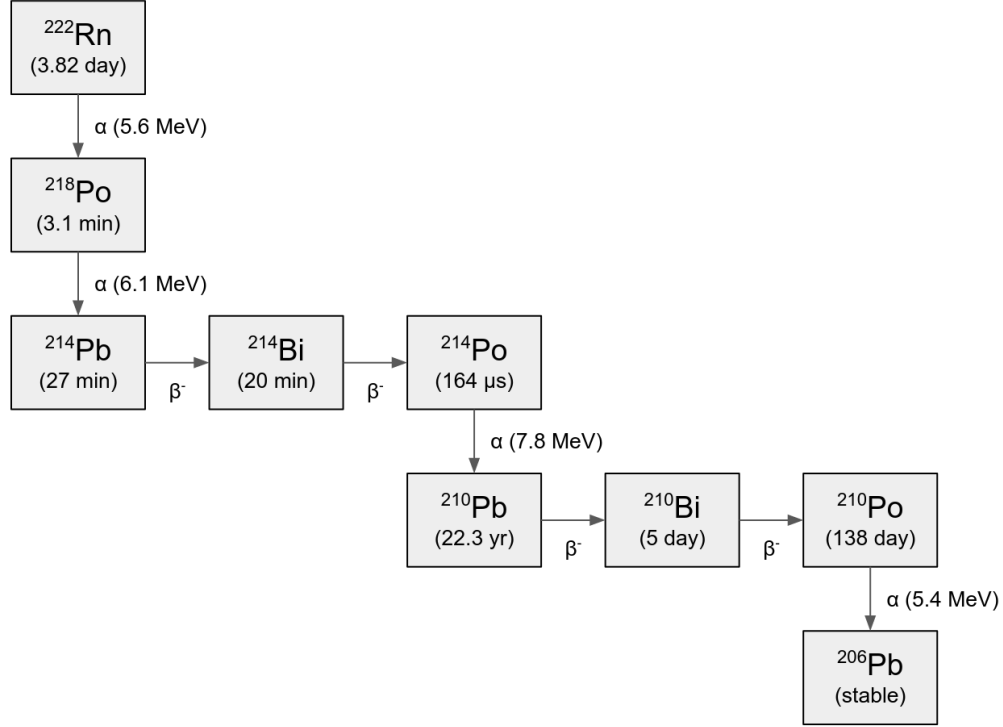


Figure 4.1: Decay chain of ^{222}Rn . Only decays with a branching ratio greater than 99% are shown. Data obtained from Ref. [112].

of 0.3 μs . The second path is an initial α decay to ^{208}Tl , followed by a β emission. It is important to note that ^{208}Tl does not have “naked” β decay modes and the accompanying γ rays generally lead to MS classification. Therefore, the only β source that contributes significantly to $0\nu\beta\beta\phi$ searches is ^{212}Pb .

Other than being an important background source, the relatively short half-lives of ^{220}Rn and its progeny provide an opportunity to calibrate the detector for its continuous ER responses. This calibration was not performed with a large scale prior to the collection of the SR1 dataset. At the time of this work, the ^{220}Rn calibration has been performed under detector conditions tuned for later data taking. The remainder of this chapter focuses on the ^{222}Rn decay chain, especially on the ^{214}Pb progeny. This choice is made because of its higher activity, but also the limited amount of ^{220}Rn events in the initial set of LZ data.

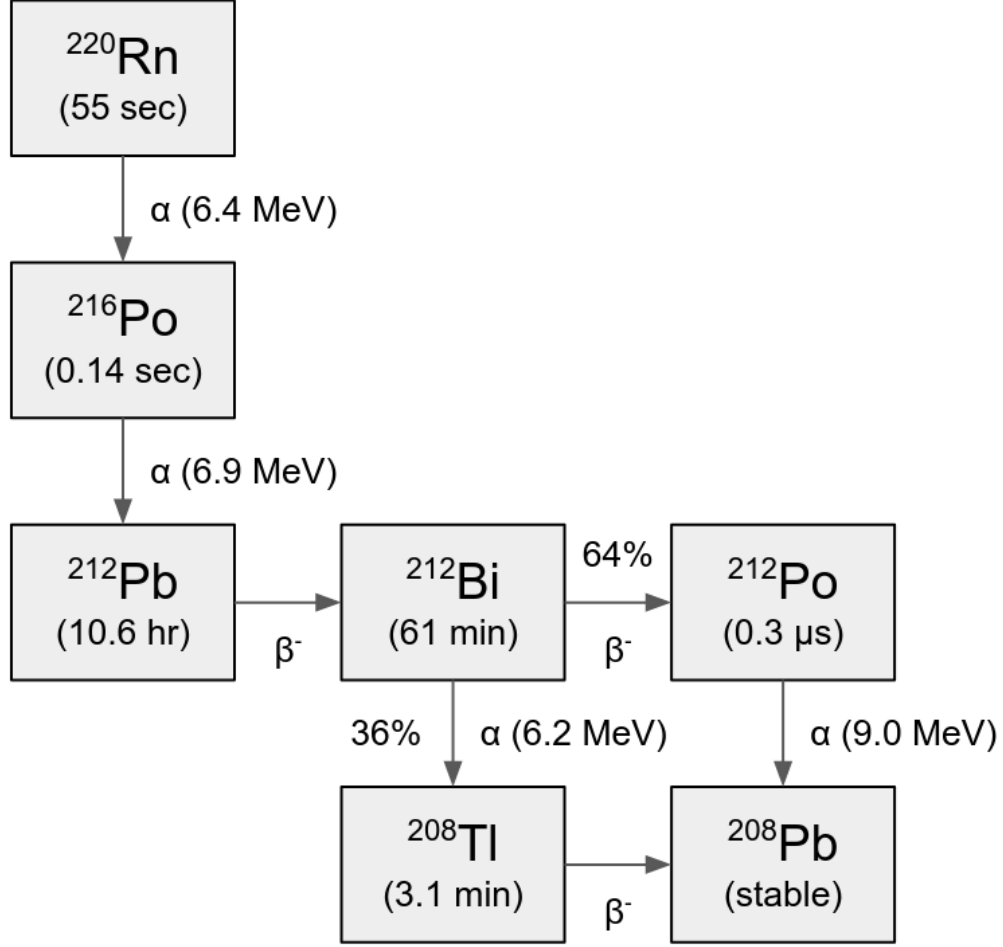


Figure 4.2: Decay chain of ^{220}Rn . Only decay branches with a branching ratio greater than 99% are shown. Data obtained from Ref. [112]

4.2 Spatial Non-uniformity of Radon Progeny

The sensitivity projection presented in Chapter 3 assumes spatial uniformity for all internal radioactive sources, including all radon progeny, within the active LXe volume. This assumption held in previous generation experiments with LXe mass at the tonne-scale or below, where turbulent mixing was difficult to prevent, resulting in a uniform dispersion of internal radioactive sources. With the potential target of isolating radon contaminants in mind, LZ is designed to deliver sub-cooled liquid at the bottom of the TPC, have the ability to control the thermal profile, and have a skin that thermally protects the TPC. These features enable LZ to actively modify the flow patterns of LXe and potentially impact the

spatial distribution of radon and its progeny in the TPC. This is also helped by the large active LXe masses in LZ, requiring much longer time periods for complete circulation and mixing. Deviations from spatial uniformity may induce FV-dependent isotopic activities of radon progeny, which in turn can affect the background model and sensitivity projections.

Examining the level of spatial non-uniformity requires the selection of a pure population of radon progeny events. For many of the radon progeny isotopes, this can be achieved by tagging the α decays with the known energy through their extremely large S1 signals, which are very distinctive from other backgrounds. One can take a classification-agnostic approach as illustrated in the comprehensive background determination analysis for LZ [2]. This approach selects all events with S1 areas within the expected range, regardless of their event classification. It is sensitive to more populations and provides a more complete dataset of the radon progeny of interest, including those that are not classified as SS due to reasons such as missing S2 signals for near-wall events. The drawback of this approach is evident: there is no guarantee that the selected events will have an S2 signal for position and energy reconstruction. Energy reconstruction can still be achieved using just the S1 area, and position reconstruction can be partially performed in z direction by leveraging the top-bottom asymmetry (TBA) of the S1 signals even in the absence of S2. This quantity is defined as the difference between the S1 light collected by the top and bottom PMT arrays, divided by the total S1 light collected. However, reconstruction of the x, y position cannot be performed without the PMT hit patterns of the S2 signal. Therefore, the classification-agnostic approach is mainly used for determining the activity of the radon progeny, while an SS-only analysis provides more information to the position distribution study. Given the focus of this study is the FV-dependent activity of ^{214}Pb , the SS-only approach is adopted.

The spatial distribution of ^{222}Rn is obtained as a starting point to assess the uniformity of progeny further down the decay chain. The study utilises a considerable fraction of the SR1 dataset, with an accumulated live-time of 17.5 days. After applying an SS-only analysis cut, the recorded events are plotted in the parameter space with the z position against the corrected S1 area (S1c). Within the range of S1c shown in Figure 4.3, two prominent bands

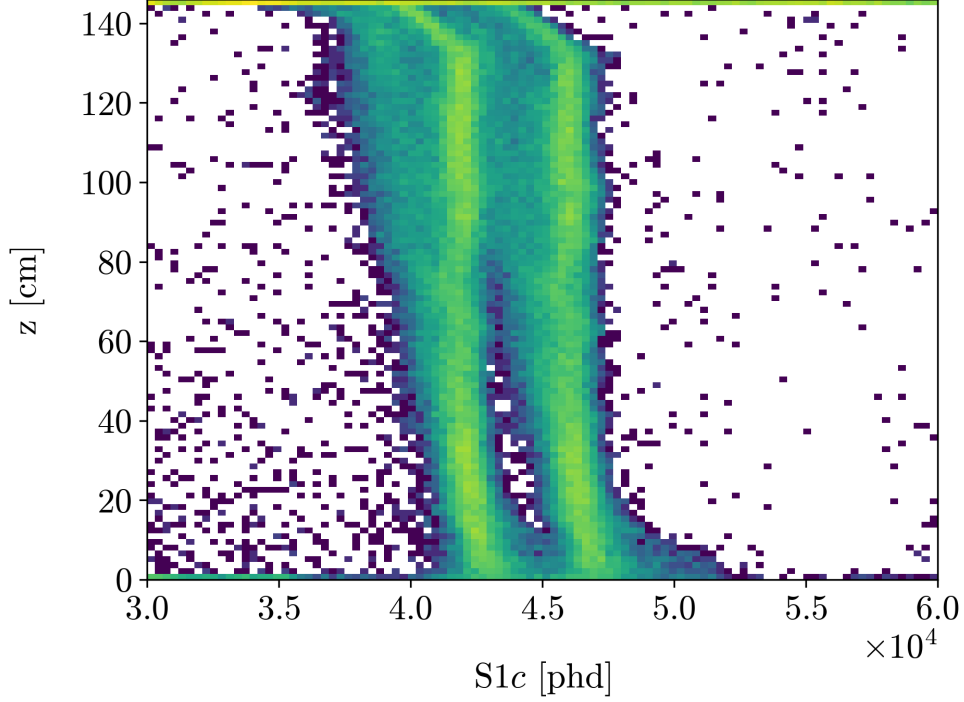


Figure 4.3: The bands of ^{222}Rn and ^{218}Po α decays, with corrected S1 ($S1c$) measured in units of photons detected (phd). The middle of the bands are vertical, indicating good S1 correction. The top and bottom of the TPC have less well corrected S1 signals, possibly due to light collection efficiency. There is also smearing of the bands, leading to a small degree of overlap.

of events are observed. The band with a lower $S1c$ corresponds to the 5.6 MeV α emission from ^{222}Rn , while the higher energy band corresponds to the 6.1 MeV α emission from ^{218}Po . The bands are nearly vertical in the middle section of the TPC, but deviate at the top and the bottom. There is also evident smearing of the bands in the top half of the TPC as the default LZ S1 correction algorithm was not tuned for these large α energies at the time of this analysis. (Note that significant work has been done on the S1 correction algorithm since then and the smearing should be less prominent in future science runs.) The smearing results in a small degree of overlap between the two bands, meaning that a simple analysis cut is likely to lead to some leakage of events from one band to the other.

An analysis cut is designed to contour the ^{222}Rn band in the parameter space, selecting a

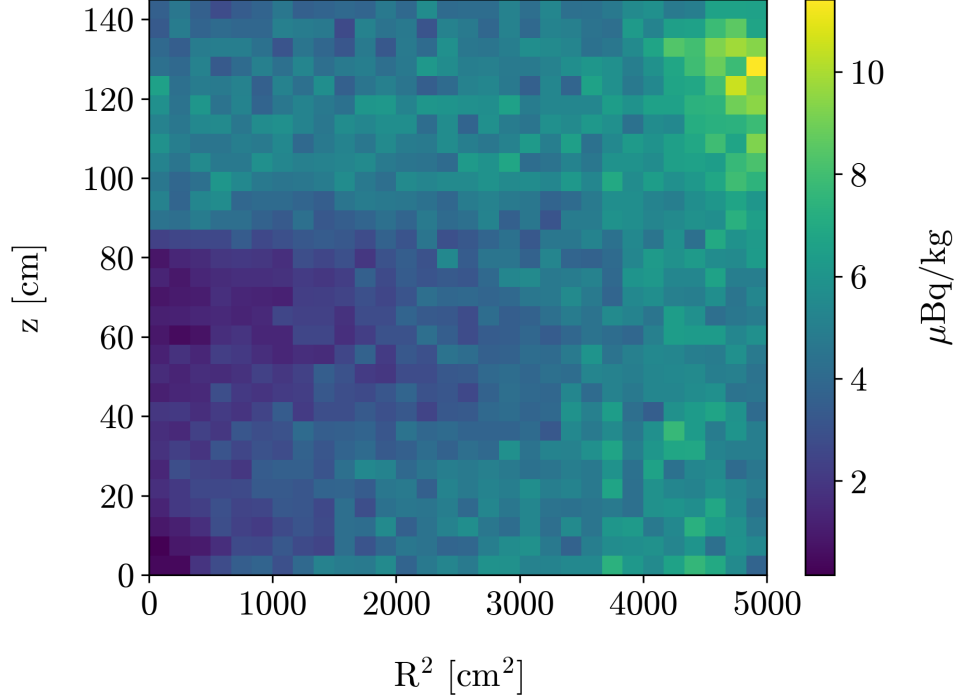


Figure 4.4: The observed spatial distribution of ^{222}Rn in SR1. There is a clear central “slow-mixing” region with lower activity. The top side of the detector shows higher activity due to leakage of ^{218}Po events into the selection cuts.

relatively pure ^{222}Rn population with few events from the overlap region between the bands. The position distribution of the selected population can then be investigated in the parameter space of z against R^2 , as illustrated in Figure 4.4. It is evident that there is some leakage of events from the ^{218}Po band around the edge of the top of the detector, though the effect is relatively small on the overall spatial distribution of the selected events. The figure reveals a highly non-uniform position distribution of ^{222}Rn , which was not observed in previous-generation LXe TPC experiments. There is a “slow-mixing” inner region with considerably lower ^{222}Rn event rate than the rest of the TPC. This observation confirms the ability of LZ to isolate radon contaminants in the active volume before complete mixing.

The quiet inner region is almost entirely encompassed in the optimised $0\nu\beta\beta\phi$ FV as obtained in the previous chapter. Since the $0\nu\beta\beta\phi$ FV is generally smaller than the SR1 WIMP FV, the average ^{222}Rn decay rate within the $0\nu\beta\beta\phi$ FV is weighted closer to the decay rate in the

slow-mixing region. Therefore, for the ^{222}Rn isotope, the activity per unit LXe mass within the $0\nu\beta\beta\phi$ FV should be lower than that in the full SR1 WIMP FV. The same statement cannot be made for all radon progeny though, as they may each individually have a different distribution within the TPC.

4.3 ^{214}Pb Tagging with Multiple Scatters

The confirmed non-uniformity of ^{222}Rn in the LZ TPC means that its progeny, including ^{214}Pb , cannot be assumed to be uniformly dispersed. As a β emitter in the radon chain, ^{214}Pb is a significant internal background source for ER events. In the context of $0\nu\beta\beta\phi$ searches, ^{214}Pb is particularly important for the low energy side of the background model. Even though the energy-only sensitivity projection of $0\nu\beta\beta\phi$ modes does not rely on position distribution of background sources, it is crucial to understand the relative activity of ^{214}Pb in the $0\nu\beta\beta\phi$ FV in comparison to the entire active LXe volume. This allows for energy PDFs to be scaled accordingly, ensuring a more accurate background model.

Table 4.1: Prominent β decay modes of ^{214}Pb . Only decay branches with a branching ratio greater than 1% are shown. The subscripts of the decay mode notation specifies the initial and final nuclear states of the decay. Data obtained from Ref. [111].

Mode	E_{avg} (keV)	E_{end} (keV)	Intensity (%)
$\beta_{0,9}^-$	48.0	179	2.75
$\beta_{0,5}^-$	205.1	666	44.5
$\beta_{0,4}^-$	225.3	723	39.0
$\beta_{0,0}^-$	334.5	1018	12.7

Table 4.1 provides a list of the ^{214}Pb β decay modes with significant branching ratios (BR > 1%). The decay modes that end up in excited nuclear states of ^{214}Bi are accompanied by γ emissions, leading to events that are expected to be reconstructed as MS. However, the “naked” $\beta_{0,0}^-$ mode, whereby the ^{214}Pb ground nuclear state decays directly to the ^{214}Bi ground nuclear state, has no accompanying γ emission. These events are expected to be

Table 4.2: Prominent γ decay modes of ^{214}Pb . Only decay branches with a branching ratio greater than 0.5% are shown. The subscripts of the decay mode notation specifies the initial and final nuclear states of the decay, with data obtained from Ref. [111]. The expected classification and the number of separable S2 signals (n_{S2}) in such decay events are also listed.

Mode	E (keV)	Intensity (%)	Expected Classification (n_{S2})
$\gamma_{4,1}$	242	7.26	MS (2)
$\gamma_{4,0}$	295	18.47	MS (2)
$\gamma_{5,0}$	352	35.72	MS (2)
$\gamma_{9,1}$	786	1.06	MS (>2)
$\gamma_{9,0}$	839	0.58	MS (>2)

reconstructed as SS and contribute significantly to the background for $0\nu\beta\beta\phi$ search.

While there is a lack of an efficient direct tagging method for $\beta_{0,0}^-$ events in ^{214}Pb , its position distribution can still be inferred from the other decay branches. This is based on the assumption that the decay mode of a ^{214}Pb nucleus undergoes is independent of its position within the TPC. If any one of the decay branches can be tagged and its position distribution inferred, the same distribution can be applied to all decay branches of ^{214}Pb .

A possible method of tagging a pure population of ^{214}Pb decay branch is to look for the accompanying γ lines with known energies. Table 4.2 provides a list of the relevant γ decay modes of the ^{214}Bi nucleus that immediately follows the ^{214}Pb β decay. Among these branches, the $\gamma_{5,0}$ mode seems to be the most promising for tagging. Many events from this decay mode are expected to be reconstructed as MS with two distinct S2s, one from the β and the other from the 352 keV γ emission. This is subject to the condition that the γ -ray travels a sufficient vertical distance from the β decay site, allowing the two S2 signals to be resolved. This condition is likely to be met, as the dominant electromagnetic process in LXe in this energy range is Compton scattering, with a mean free path of $\mathcal{O}(\text{cm})$. The $\gamma_{4,1}$ and $\gamma_{4,0}$ modes with energies 295 keV and 242 keV, respectively, are also potential options for

tagging, although they have lower relative intensities when comparing to the $\gamma_{5,0}$ mode.

One possible bottleneck associated with this approach is the energy resolution. In the case of a ^{214}Pb decay, the time separation between the β and the γ emission is very small, resulting in scintillation photons from both emissions arriving at the PMT arrays almost simultaneously and form a single S1 signal. Therefore, energy reconstruction of the γ photon is based on the S2 signal only, leading to a degraded energy resolution and causing overlaps between the γ peaks. Furthermore, the β decay of ^{214}Pb has a continuous energy spectrum below its Q-value, which overlaps with the γ lines. Therefore, the S2 signal associated with the γ emission cannot be easily identified by comparing the relative sizes of the two S2s.

The challenges associated with energy resolution and overlapping energy spectra of the γ peak and β continuum can be potentially resolved by tagging the $\gamma_{9,0}$ or the $\gamma_{9,1}$ mode. These modes have γ energies of ~ 800 keV, which are far above the 179 keV Q-value of the $\beta_{0,9}^-$ mode. Also, the large S2 from the γ emission helps to improve energy resolution from S2-only energy reconstruction. The feasibility of identifying these populations in real data was cross-checked by looking at the fast chain simulation of ^{214}Pb and its progeny. This was performed by examining the energy deposition of each vertex in the MCTruth information of ^{214}Pb simulation. It is important to note that this energy deposition does not correspond to the reconstructed energy, as the MCTruth information is based on GEANT4 vertices only and does not take into account detector parameters that requires processing by NEST. Therefore the energy desposition spectrum plot from the MCTruth information should contain more peaks than those expected in a reconstructed energy spectrum.

Figure 4.5 shows the energy deposition spectrum from the MCTruth information. The peaks that correspond to the lower energy γ modes (< 400 keV) are clearly visible, but there are no visible peaks at energies corresponding to the $\gamma_{9,0}$ and $\gamma_{9,1}$ mode. This can be attributed to the relatively low combined intensity of these two γ modes at 1.64%. In addition, the energy scale of these two decay modes is highly Compton-dominated, with a high probability that the γ photon deposits energy into multiple S2 signals. Without the information of which

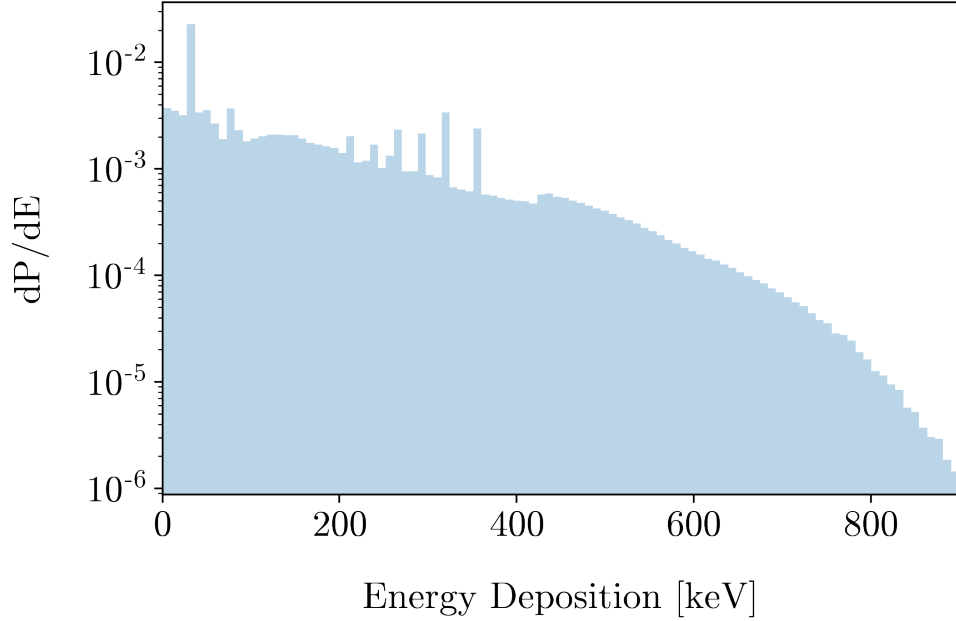


Figure 4.5: Simulated energy deposition of ^{214}Pb decay in LXe. The histogram takes into account energy deposition at all simulated GEANT4 vertices, without applying any analysis cut.

S2 signal corresponds to the energy deposition of the γ photon, it is infeasible to design a selection criteria for the $\gamma_{9,0}$ and $\gamma_{9,1}$ modes even if the condition of having exactly two S2s signals is relaxed. As a result, the γ mode that are prioritised in this analysis remain $\gamma_{5,0}$, $\gamma_{4,0}$ and $\gamma_{4,1}$.

The study on ^{214}Pb simulation continues by utilising the NEST-processed RQs and applying a simple set of cuts based on the nature of the non-naked β decay modes. The events of interest should be reconstructed as MS, as well as having exactly two S2s from the β and the accompanying γ emission. To tag the γ mode, it is necessary to distinguish between the S2 signal from the γ emission and that from the β emission. One naive approach is to use the time information within an event, assuming that the γ emission always takes place after the β . However, the time information for the S2 signals only reflects their arrival time at the PMT array, which is an indication of depth rather than the chronological order of the decays.

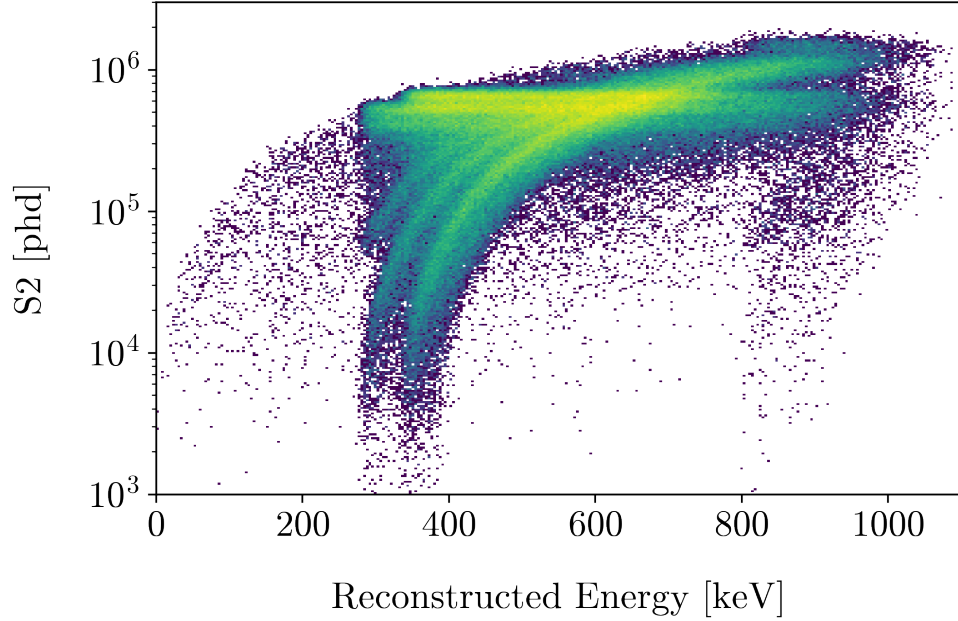


Figure 4.6: Simulated ^{214}Pb β and γ bands in the ^{214}Pb tagging parameter space, with S2 measured in units of photons detected (phd). Each event has two S2s corresponding to the same total reconstructed energy. Events that have one S2 in a β band should also have the other S2 in the corresponding γ band.

Instead, one can examine the parameter space as illustrated in Figure 4.6. For each event, the areas of both S2s are plotted against the total reconstructed energy of the event. The energy reconstruction formula is slightly adapted for MS, with the S2 in Eq. 2.14 replaced by the sum of the two S2 areas. From the figure, it is evident that the S2s split into two classes of bands: the γ bands, which remain constant in S2 area regardless of the total reconstructed energy of the event; and the β bands, which increase linearly with the total reconstructed energy. Since the β emission has an energy continuum that extends from the Q-value down to very low energy, the minimum total reconstructed energy of a β band corresponds to the γ energy.

The band structure in Figure 4.6 agrees nicely with expectations. There are three distinguishable β bands that extrapolate to the expected reconstructed energy, corresponding to the $\gamma_{5,0}$, $\gamma_{4,1}$ and $\gamma_{4,0}$ modes. The γ bands are less well separated due to the relatively poor

S2-only energy resolution, but three distinguishable horizontal bands are still visible in the figure. The β bands are well separated from the γ bands, as well as from each other, below ~ 500 keV of reconstructed energy. In the energy range between 500 keV and 700 keV, the β bands intersect with the γ bands, indicating that the two S2s from β and γ are indistinguishable. Above 700 keV, the β bands almost merge with each other. This merging of bands makes it almost impossible to identify which γ mode the event belongs to and thus makes it inseparable from other background events in this energy range. Therefore, the ability to tag a ^{214}Pb decay mode from the accompanying γ emission lies in the lower end of the energy spectrum, where the β bands and γ bands are well separated and distinguishable.

The methodology of ^{214}Pb tagging with MS has been verified with the simulation, but it needs to be further tested with real data. The full SR1 dataset of LZ is utilised to check the performance of the tagging methodology. Only events that are classified as MS and have exactly two S2s are selected. As γ rays from detector material and the external cavern are expected to induce many MS events in the dataset, a further FV cut is applied to focus on ^{214}Pb and other internal backgrounds. This FV is defined as the inner one-tonne cylindrical volume with $r \leq 45$ cm and $35 \text{ cm} \leq z \leq 95$ cm. The position coordinates of an event are taken as the weighted average of reconstructed x , y , and z coordinates of the two S2s, with the weights being the ratio of the individual S2 area to the sum of the S2s.

The events that pass the cuts are then plotted in the S2 vs. reconstructed energy parameter space, as illustrated in Figure 4.7a. It can be observed that the ^{214}Pb β and γ bands are visible but not well separated. The more troublesome feature in this plot is the appearance of two vertical bands of populations at around 200 keV and 400 keV. These populations span the majority of energy range where the β bands are separable, thus severely impeding the ^{214}Pb tagging capability.

Since the above SR1 analysis was restricted to the inner one-tonne FV, the additional populations that appeared must come from an internal background source within the bulk LXe. Considering the common radioactive isotopes and their distribution in the parameter space

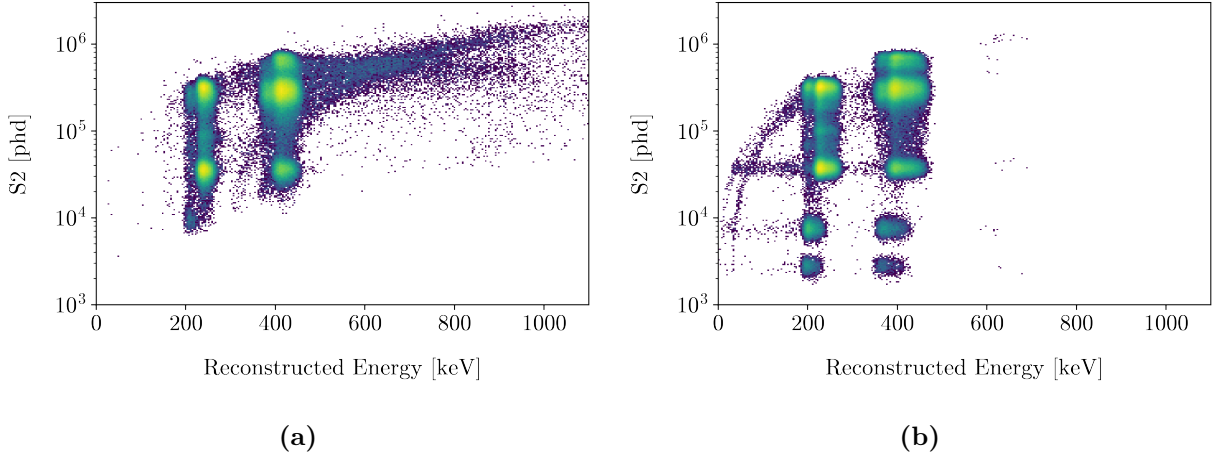


Figure 4.7: Comparison of SR1 dataset and simulated ^{127}Xe events in the ^{214}Pb tagging parameter space. **(a):** SR1 dataset in the ^{214}Pb tagging parameter space. The ^{214}Pb β and γ bands are barely visible, and there exist additional populations in the lower end of the energy spectrum. **(b):** Simulated ^{127}Xe events in the ^{214}Pb tagging parameter space. The events clearly resemble the observed populations in the SR1 dataset.

of interest reveals the origin of this population. It is evident that the additional populations seen in the SR1 dataset resembles similar distribution as one would expect from ^{127}Xe simulation, as shown in Figure 4.7b. During the storage and transportation of xenon prior to being brought underground, cosmogenic xenon backgrounds are produced, including ^{127}Xe . The activation process is suppressed when the xenon is shielded underground as a result of the rock overburden. Without the source of production, the activated xenon isotopes are expected to be negligible in the long term. However, the time between the last delivery of xenon to SURF and the start of SR1 is less than four months, which is not sufficient for some activated isotopes to decay away. With a relatively long half-life of 36.4 days, a significant fraction of ^{127}Xe is expected to be prevalent during SR1. The presence of ^{127}Xe in the SR1 dataset introduces challenges to the ^{214}Pb tagging methodology. As illustrated in Figure 4.8, the ^{127}Xe nucleus decays via two electron capture modes $\epsilon_{0,2}$ and $\epsilon_{0,3}$ to ^{127}I . The decay leaves the ^{127}I in excited nuclear states, leading to subsequent γ ray emission, with $\gamma_{3,2}$, $\gamma_{2,0}$, $\gamma_{3,0}$ being the major branches. Meanwhile, the electron structure rearranges itself to fill the hole left by the captured electron, causing the emission of characteristic X-rays or a cascade of Auger electrons in the process.

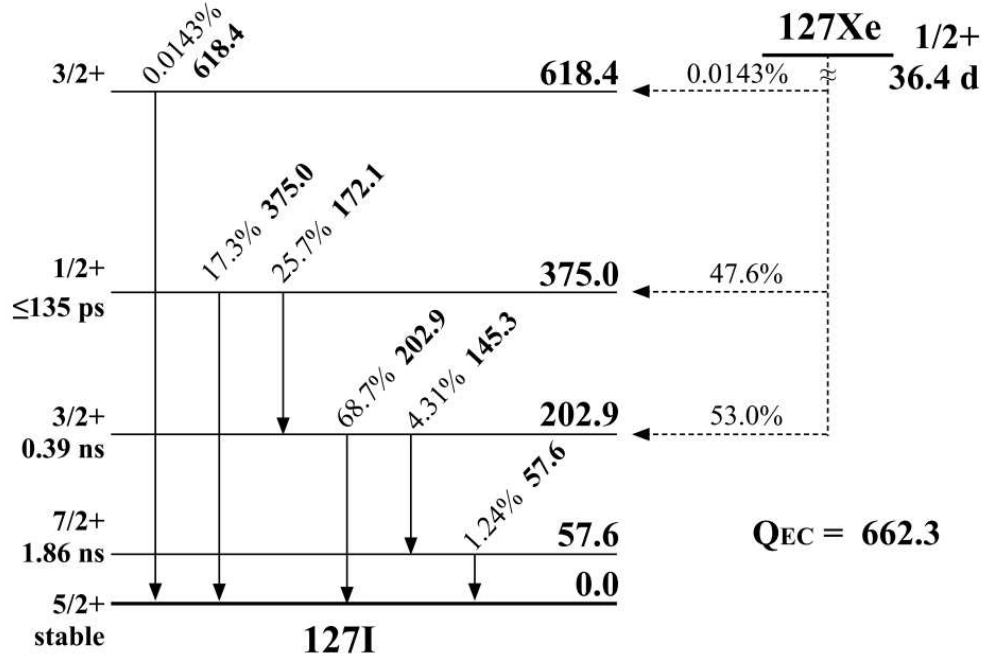


Figure 4.8: Decay scheme of ^{127}Xe electron capture to ^{127}I and the subsequent γ emission [111].

For the γ emission, only prominent branches with intensity greater than 1% are included. The decay energies are in units of keV. The figure is taken from Ref. [120].

While the X-ray and Auger electrons have short mean free paths in LXe, the γ photons can deposit energy sufficiently far away to be identified as a separate interaction site, leading to MS events. This results in two bands of events in the reconstructed energy spectrum. The first band has a total energy deposition of ~ 200 keV that corresponds to the $\epsilon_{0,2}$ electron capture mode, with the main S2 populations being the $\gamma_{2,0}$ at 172 keV and the ~ 30 keV X-ray. The second band is at ~ 400 keV, corresponding to the $\epsilon_{0,3}$ electron capture mode. The excited nuclear state of ^{127}I produced by this mode mainly takes two decay paths: either the $\gamma_{3,0}$ decay mode that ends directly in the ground state, or the $\gamma_{3,2}$ to an intermediate excited state, followed by the $\gamma_{2,0}$ to the ground state. Therefore, the band consists of three main populations of S2s: the $\gamma_{3,0}$ at 375 keV, the ~ 30 keV X-ray and an overlapped population from the $\gamma_{3,2}$ at 172 keV and the $\gamma_{2,0}$ at 203 keV.

Together, the two vertical bands of ^{127}Xe events in the ^{214}Pb tagging parameter space mask

the energy range where the ^{214}Pb β bands are separable. Even if one restricts the analysis to the second half of SR1, where the ^{127}Xe activity has reduced significantly, the remaining ^{127}Xe still heavily contaminates the dataset for the purpose of ^{214}Pb tagging. The narrow gap between the two bands leaves very little scope to obtain enough statistics of ^{214}Pb events. The tagging methodology can work in principle, and is worth further investigation in future data taking, when the remaining ^{127}Xe activity has decayed away sufficiently. As of analysis with SR1 dataset though, it is not feasible to obtain a purely data-driven position distribution of ^{214}Pb from this approach.

4.4 ^{214}Pb Position Distribution Simulation

The prevalence of ^{127}Xe during SR1 results in the MS tagging of ^{214}Pb being infeasible at the time of this work. An alternative approach is needed to obtain the ^{214}Pb position distribution, allowing for the study of its impact on LZ's sensitivity to $0\nu\beta\beta\phi$. A reasonable strategy is to adopt the same approach as that used for the background determination in LZ's SR1 WIMP search [2], with adaptations made for $0\nu\beta\beta\phi$ where necessary. The approach utilizes the α -emitting isotopes that precede and follow the ^{214}Pb β decay in the ^{222}Rn chain to indirectly derive constraints on the ^{214}Pb position distribution, supplemented with toy Monte Carlo simulations.

The central idea of the approach is to track the movement of radioactive daughter nuclei along the decay chain of ^{222}Rn . As described previously in Section 4.2, the spatial non-uniformity of ^{222}Rn can be inferred by selecting events with characteristic large S1 signals. This holds true for some other isotopes in the ^{222}Rn decay chain, including ^{218}Po and ^{214}Po . Given that the motion of radioactive nuclei evolve continuously as they progress along the decay chain, the position distribution of ^{214}Pb should be an intermediate state that is constrained by the distribution of ^{218}Po and ^{214}Po .

The position distribution of ^{218}Po can be obtained by tagging the characteristic large S1 signals as illustrated previously in Figure 4.3. Comparing the position distribution of ^{218}Po ,

as shown in Figure 4.9, with that of ^{222}Rn in Figure 4.4 shows little difference (except for the small leakage at the top of the TPC). This is expected since the half-life of ^{218}Po is only 3.1 minutes, allowing for minimal movement of the daughter nuclei from the decay site of their parent nuclei. However, the position distribution of ^{214}Po , as illustrated in Figure 4.10, deviates significantly from the previous isotopes, exhibiting a clear tendency of motion towards the bottom of the TPC. This general downward motion is due to the production of a positively charged ion in the radon-chain decay, a phenomenon that was first measured by EXO-200 in the context of liquid noble gases [121]. The electric field in LXe drifts the charged ions towards the cathode grid. The daughter nuclei inherit the existing spatial non-uniformity of the parent nuclei and the ion drift defines the subsequent position distribution the daughter nuclei.

The relationship between the relevant charged progeny and their corresponding ion fractions are illustrated in Figure 4.11. There are three decay steps of interest, starting from ^{222}Rn and reaching the ^{214}Bi nuclei. Each decay step has the potential to produce both charged and neutral daughter nuclei, regardless of the charge on the parent nuclei. Associated with the decay steps is the fraction of charged ion produced that needs to be determined. The fraction of ^{222}Rn atoms decaying into $^{218}\text{Po}^+$ ions, denoted as f_1 , has a measured value of 0.46 ± 0.04 in SR1 [2]. This measurement can be obtained by tagging a population of ^{222}Rn - ^{218}Po pairs and identifying the ones with the daughter ^{218}Po drifted downwards. The average velocity of the ions was also measured, resulting in an ion mobility of $0.242 \pm 0.031 \text{ cm}^2/(\text{kV} \cdot \text{s})$. This measurement is in agreement with the previous literature value of $0.219 \pm 0.004 \text{ cm}^2/(\text{kV} \cdot \text{s})$ reported by EXO-200 [121].

The charged ion fraction of ^{214}Pb is more complicated due to the existence of both neutral ^{218}Po atom and charged $^{218}\text{Po}^+$ ion parent nuclei. The probability of neutral ^{218}Po decaying into charged $^{214}\text{Pb}^+$, denoted f_{2a} , is assumed to have the same value as f_1 . This assumption is supported by the fact that Po and Pb nuclei have comparable first ionisation potentials at 8.4 eV and 7.4 eV, respectively. In addition, the energy carried by the α emission from the ^{222}Rn and ^{218}Po isotopes are also very similar, at 6.3 eV and 6.8 eV respectively. Therefore,

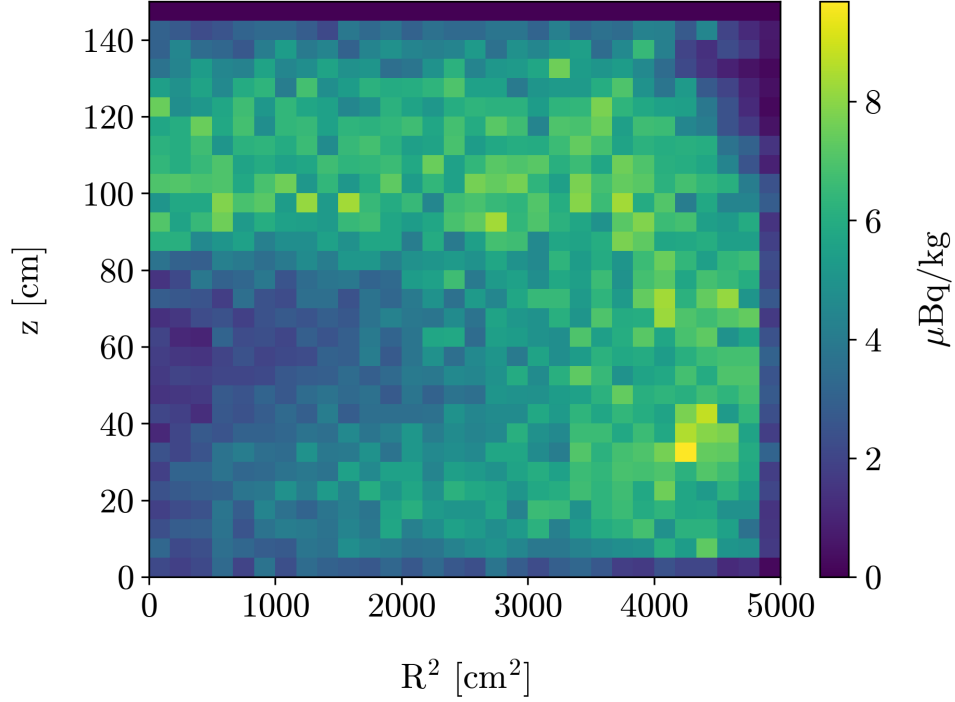


Figure 4.9: The observed spatial distribution of ^{218}Po in SR1. The distribution resembles similar characteristics to the observed ^{222}Rn distribution as shown in Figure 4.4, with a clear central “slow-mixing” region with lower activity. The similarity is expected due to the short 3.1 min half-life of ^{218}Po , leading to insignificant ion drift distance. The top side of the detector shows lower activity due to leakage of events into the ^{222}Rn selection cuts.

it is assumed that the α particle from both decays have nearly identical probabilities to ionise the decay product and produce a singly positive ion, a conclusion that was also reached by the EXO collaboration [121]. In the case of $^{218}\text{Po}^+$ ion decay, the charged progeny fraction f_{2b} is assumed to be double the value of f_{2a} . This is because the $^{218}\text{Po}^+$ ion decay leaves only one extra free electron in the vicinity of $^{214}\text{Pb}^+$, rather than two extra electrons as in the case of the ^{218}Po atom. The chance for the produced $^{214}\text{Pb}^+$ ion to be neutralised by the free electrons is therefore halved, leading to twice the charged ion fraction. For the third decay stage from ^{214}Pb or $^{214}\text{Pb}^+$ to $^{214}\text{Bi}^+$, the literature value of $f_3 = 0.763$ is adopted [121].

The motion of radon progeny atoms and ions are simulated using a toy Monte Carlo model.

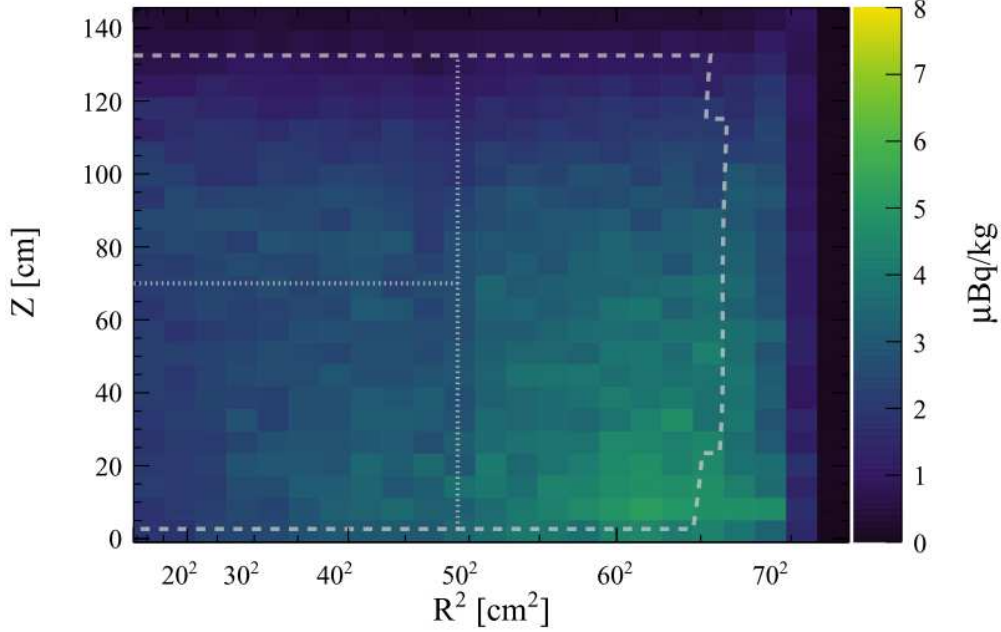


Figure 4.10: The observed spatial distribution of ^{214}Po in SR1. Figure taken from Ref. [2]. The outer dashed lines represents the SR1 WIMP search FV, which is further divided into upper, lower and outer regions by the inner dashed lines. The lower region here corresponds to the “slow mixing” region observed in ^{218}Po distribution in Figure 4.9.

The simulation assumes only the vertical motion of ions, influenced by the electric field in LXe. In practice, this is not entirely accurate. The thermodynamic condition and the injection of circulated xenon induces a flow pattern in the LXe bulk, leading to motion of neutral atoms up and down the TPC. However, the speed of this neutral atom flow is approximately an order of magnitude lower than that of the ion drift and is therefore neglected [2].

The simulation begins with the position distribution of ^{218}Po events as obtained previously in Figure 4.9. Each event then has a probability to be assigned either a charged tag or a neutral tag, based on the ion fraction f_1 . The atoms and ions are allowed to evolve over time and decay according to a Poisson distribution, generating a simulated position distribution of ^{214}Pb as shown in Figure 4.12. At this stage, the events are assigned a new charge or neutral tag based on the parent nuclei and the corresponding ion fraction. The position coordinates of the nuclei are then allowed to evolve further, leading to a simulated position distribution of ^{214}Bi . Since the signature Bi-Po events are nearly instantaneous due to the

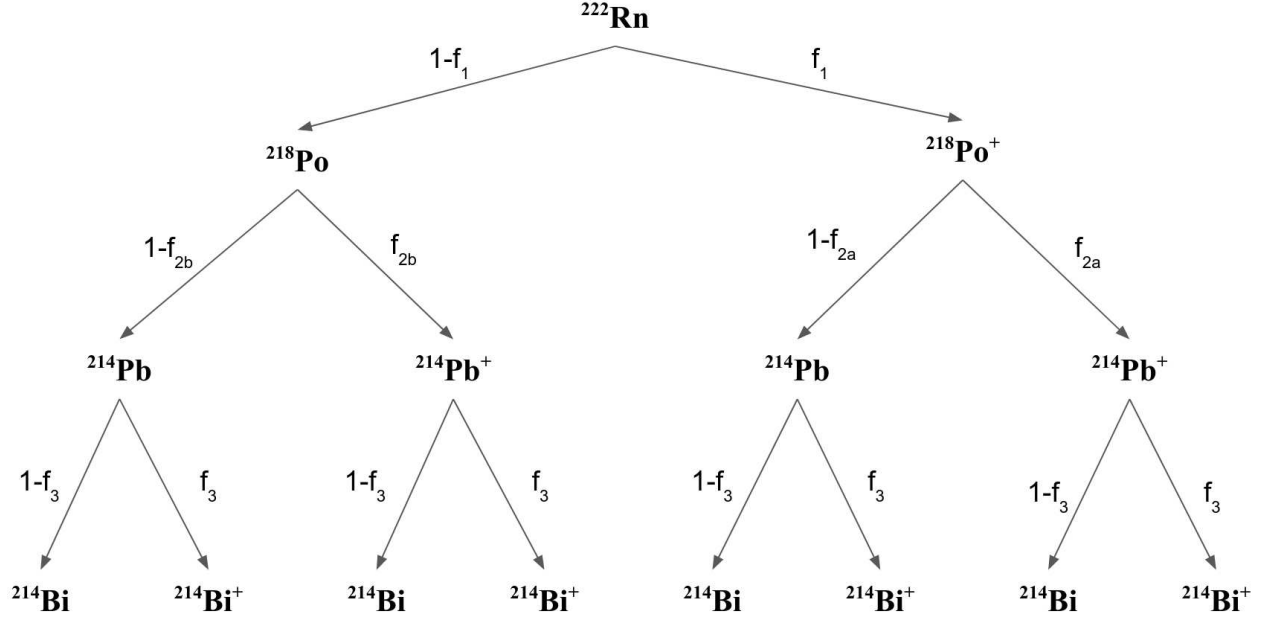


Figure 4.11: Illustration of ion fraction along decay paths of ^{222}Rn . Each path is provided with an experimentally determined probability.

164 μs half-life of ^{214}Bi , the position distribution of ^{214}Bi should be nearly identical to ^{214}Po . In SR1, the validity of this toy Monte Carlo simulation has been cross-checked by comparing the simulated distribution of ^{214}Po with the observed distribution in SR1 data, which shows good agreement[2].

4.5 Impact on the Sensitivity to $0\nu\beta\beta\phi$

The rate of ^{214}Pb decays within the $0\nu\beta\beta\phi$ FV can be estimated from the simulated position distribution. Assuming an initial average activity of 3.26 $\mu\text{Bq/kg}$ as measured in SR1, the analysis is performed by comparing the number of events per unit volume within the $0\nu\beta\beta\phi$ FV and that of the SR1 WIMP FV. For the largest $n = 7$ $0\nu\beta\beta\phi$ FV, the estimated ^{214}Pb activity is 3.22 $\mu\text{Bq/kg}$, and for the smallest $n = 1$ FV, the activity is 3.30 $\mu\text{Bq/kg}$. Both of these values differ less than 2% from the reported activity in the SR1 WIMP FV and are within uncertainty of the estimate.

Unlike the observed position distribution of ^{218}Po , the activity of ^{214}Pb does not benefit

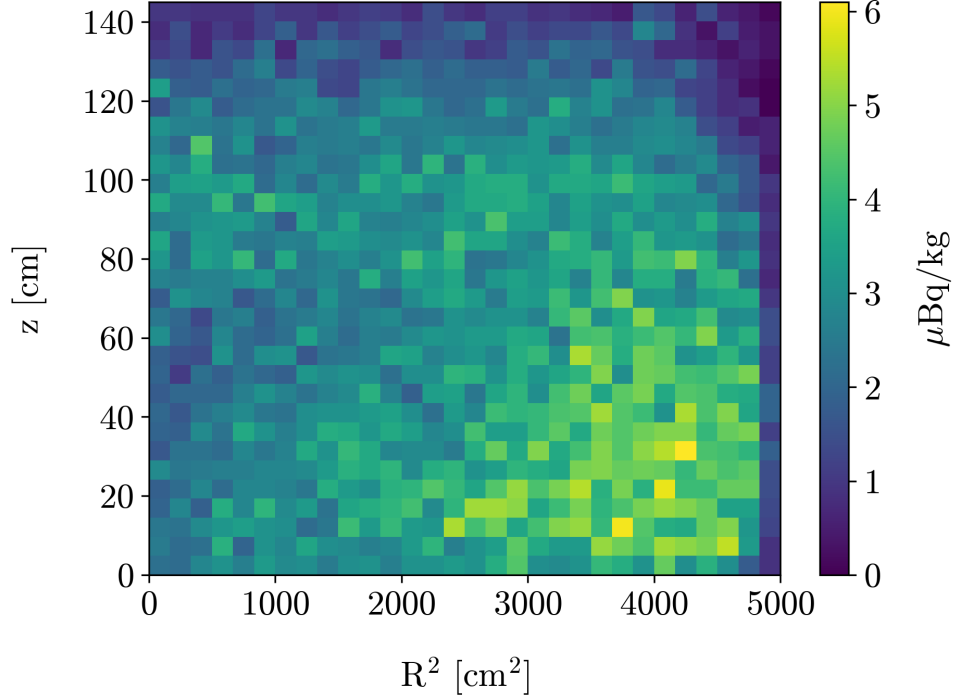


Figure 4.12: Simulated spatial distribution of ^{214}Pb . The starting points of the simulation are based on the observed ^{218}Po spatial distribution.

as much from the quiet “slow-mixing” region. This should not be a surprise given that the downward drift of ions under the electric field essentially mixes the radon progeny into the “slow-mixing” region, lowering the level of inhomogeneity in the ^{214}Pb position distribution.

The spatial non-uniformity of radon progeny is a phenomenon that has only recently been observed in the multi-tonne scale xenon TPC of LZ. There remains a wide scope of study, including ways of controlling the non-uniformity to favour particular scientific objectives. At the time of writing, XENON1T has demonstrated a tagging algorithm to reduce radon-induced backgrounds [122]. LZ is active in this field and a ^{214}Pb veto algorithm using liquid flow patterns is under development within the collaboration, with preliminary results indicating a $> 50\%$ reduction efficiency. The novel tagging method based on multiple scatters developed in this work can be a powerful tool to help with the study, despite being limited by the prevalent activated xenon backgrounds in the SR1 dataset. As for the impact of the

non-uniformity on $0\nu\beta\beta\phi$ sensitivity projection, an alternative toy Monte Carlo approach to estimate the ^{214}Pb spatial distribution is adopted. The results show that, despite the significant spatial non-uniformity observed in radon, the averaged activity of ^{214}Pb in any of the $0\nu\beta\beta\phi$ FV is in fact very similar to that in the SR1 WIMP FV. Provided that the detector conditions do not change drastically in future data taking, leading to a significant variation in the spatial distribution of ^{214}Pb , the current level of spatial non-uniformity in radon progeny has no significant impact on LZ's half-life sensitivity to $0\nu\beta\beta\phi$.

Chapter 5

Search for $n = 1$ Majoron-Emitting Mode with SR1 Data

In 2022, LZ reported results from its first search for WIMPs with the Science Run 1 (SR1) dataset. The search had an accumulated exposure of 60 live days for WIMP search with a 5.5 tonne fiducial mass. Based on a PLR analysis, the results are consistent with the background-only hypothesis. The search enabled LZ to set the most stringent limits on the scattering cross sections for WIMPs with masses above $9 \text{ GeV}/c^2$.

The data acquisition approach of LZ keeps all of the data collected from events that pass the LZ triggers, including those that are later considered to be unsuitable for the WIMP search analysis. While all the calibrations and detector conditions during SR1 are optimised for the WIMP search, the accumulated data is still available for other physics searches. This chapter aims at setting an initial limit on $n = 1$ $0\nu\beta\beta\phi$ with the SR1 dataset. The analysis begins by selecting a simple set of cuts suitable for $0\nu\beta\beta\phi$ search. The cuts are then applied to both the simulation and the SR1 dataset, providing a starting point for the simulated background model to be compared with real data. The rate and the uncertainty for each component that contributes to $0\nu\beta\beta\phi$ background model is estimated, with fitting within sidebands performed where necessary, and the corresponding simulated PDFs are scaled accordingly. PLR analysis is then performed to compare the background model with SR1 data and set a half-life limit – or detection.

5.1 SR1 and Analysis Cuts

5.1.1 SR1 Data

The LZ SR1 data were collected under stable detector conditions from December 23, 2021 to May 11, 2022. The dataset was analysed for publication of LZ’s first WIMP search result [53]. During data collection, the cathode and gate grids established a uniform 193 V/cm drift field, while the anode and gate grids generated a 7.3 kV/cm extraction and electroluminescence field in the gas. The full 10 tonne xenon volume was purified through a getter system at a continuous rate of 3.3 tonne/day. This helped reach an impressive 5000 μs to 8000 μs electron lifetime against attachment to electronegative impurities, almost an order of magnitude longer than the 951 μs maximum electron drift time measured in the TPC. The DAQ trigger was set to S2 mode and recorded events within a time window of 2 ms before and 2.5 ms after the S2 signals in the TPC. Waveforms from all PMT channels in the TPC, Skin, and OD were included in the recorded events.

The summed waveform areaa from all PMT channels are measured in units of photons detected (phd), accounting for the effect of $\sim 20\%$ probability of double photoelectron from a single VUV photon for xenon luminescence light. Pulse discrimination is performed by applying filters to the summed waveforms to identify pulse boundaries. The pulses are further classified into S1 and S2 based on pulse shape and PMT hit patterns. Only the most prominent S1 and S2 pulses are used for single scatter (SS) and multiple scatter (MS) event classification based on their time ordering. The PMT hit patterns of S2 light are also used to determine the transverse location of the event using the Mercury algorithm [123]. Following tuning with uniformly dispersed calibration sources, the algorithm can achieve a 1σ spatial resolution of 4 mm for S2 signals at 3000 phd. In the vertical (z) direction, location of the event is determined by the drift time, which has a value of 0.7 mm near the cathode grid.

The identified pulses of the event undergo several corrections to normalise response within the TPC. The S1 pulses are corrected in x , y and drift time to normalise to the geometric centre of the detector. The correction mainly accounts for light collection efficiency and

quantum efficiency of different PMTs. On the other hand, the S2 pulses are normalised to the radial centre at the top of the TPC. S2 correction in the x - y plane accounts for extraction-field non-uniformity and operation status of the PMTs, while the z -direction correction is mainly due to electron attachment on impurities (i.e. electron lifetime correction). The corrected S1 and S2 values are denoted $S1c$ and $S2c$, respectively.

For the purpose of understanding detector response under continuous stable conditions, methods of bias mitigation by obscuring data were not applied during SR1 data. The collected dataset was not blinded in any parameter space, and no additional fake events (“salt-ing”) were included. While this choice allows one to focus on mitigating other potentially larger systematic errors of a new detector, it is important to keep bias mitigation in mind throughout the data analysis procedure. Most importantly, analysis cuts and preliminary background fitting are performed on sideband selections or calibration data that were taken outside the SR1 data taking period.

5.1.2 $0\nu\beta\beta\phi$ Analysis Cuts

The previous chapters consider the half-life sensitivity projection of LZ based on Monte Carlo simulations. Under the ideal quality of data assumed in the simulated dataset, the following set of cuts are applied to reach the optimal projected sensitivity:

- Single Scatter
- Skin and OD veto
- FV and ROI

The real data collected during SR1 is different from the ideal assumed by simulation. Unexpected physical phenomena within the complex environment of the detector may lead to additional particle interactions being recorded as background noise within the dataset. The analysis work presented in this chapter utilises the same version of analysis tools as the SR1 WIMP search result for consistency. Later versions of the analysis packages have since been

developed that may address some of the data quality issues, though they will only be mentioned where applicable instead of performing re-analysis. The following sections list out the analysis cuts that are identified to improve the data quality of SR1 in the context of $0\nu\beta\beta\phi$ searches.

Exclusion Periods

During the 138 calendar days between the start and end of SR1 data taking, certain periods are specifically taken by detector maintenance and calibration activity. Data collected during such periods are not included in the SR1 dataset for analysis. In addition, certain periods of data are severely affected by anomalous trigger rates (grid “hotspots”) that may flare-up for various reasons. During these periods, high signal rates are observed at localised places in the TPC. The duration of these periods is initially flagged by remote monitoring personnel during data taking, followed by validation with the collected data. Data recorded during these periods are excluded from the $0\nu\beta\beta\phi$ searches, resulting a live time loss of about 3%.

S1 and S2 Threshold

The low energy NR events that are of interest to WIMP search are required to have S1 signals with areas larger than 3 phd and at least 3-fold coincidence. Such a threshold is evidently too low in the context of high energy ER events that a $0\nu\beta\beta\phi$ search considers. In addition, the partitioning of energy into S2 signal is larger for ER events, which naturally induces the requirement for an S2 threshold cut at the same time. Motivated by the distribution of ER events in the $S1c$ and $\log(S2c)$ parameter space and their removal, an S1 threshold cut of $S1c > 100$ phd is applied to remove events with too small S1 signals, and an S2 threshold cut of $\log(S2c) > 3.5$ is chosen to remove events below the ER band in this parameter space.

Single Scatter

As the main target of SR1 is to understand the detector response for WIMP searches, the pulse clustering and event classification algorithm is tuned for low energy NR events. Since the simulations are tuned to match the general detector response under SR1 conditions, it is expected that the broad-spectrum efficiency of the cuts agrees when applied to both SR1

data and simulations. While this analysis does not attempt to re-tune the cuts for $0\nu\beta\beta\phi$ search, it is important to verify the expected agreement.

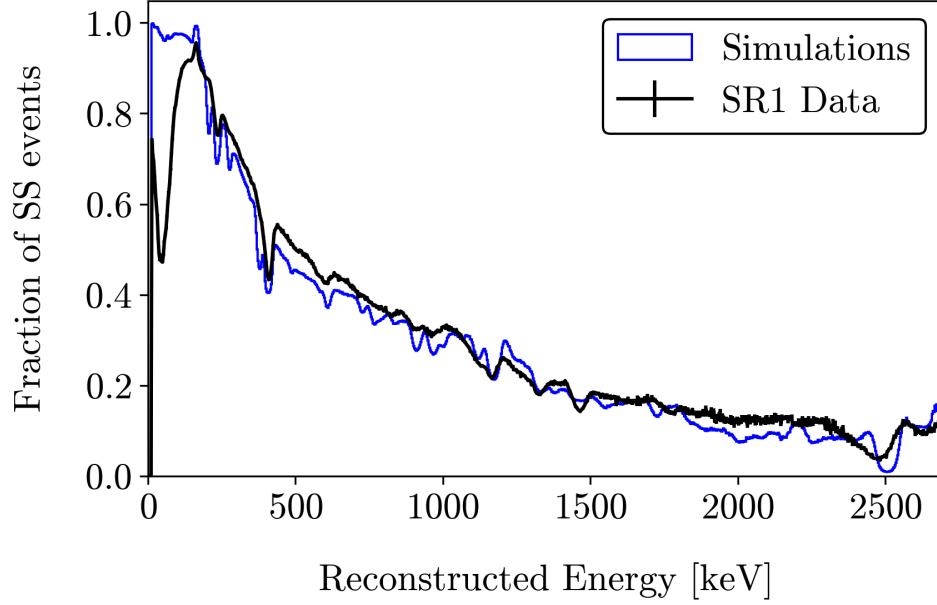


Figure 5.1: Single scatter efficiency of SR1 data and simulations. The simulations are Poisson sampled with respective scaling to match the LZ background database. These values come from prior measurements in sidebands, calibration data or screening campaign. Also included are the error bars for statistical uncertainties in SR1 data, which are very small and nearly invisible in low energy range. This is due to the large statistics of both SS and MS events in each energy bin in SR1 data.

For the single scatter efficiency, a Poisson-sampled dataset is selected from high-statistics simulations, with the activity of each component scaled to match those values recorded in the LZ background database. The fraction of events classified as single scatters in the simulation and SR1 are compared, demonstrating good agreement as shown in Figure 5.1. The deviation below ~ 200 keV is expected due to choice of only including ER sources in the sampled dataset. Also, given that energy reconstruction of MS has not been separately calibrated, the SS fraction shows a broader dip at the high-energy γ peaks than expected from the SS energy resolution. For the other parts of the spectrum, the deviations are

likely due to mismatch of component activity assumed during Poisson sampling and the real detector condition, which will be addressed later in the section with background fitting.

Skin and OD Veto

The Skin and OD veto cuts are also tuned for the SR1 WIMP search, whose position-averaged neutron tagging efficiencies have been studied with AmLi calibration sources [53]. For this analysis, the Skin and OD veto are identical to that described in the SR1 WIMP result. Any prompt skin signal within a $\pm 0.3 \mu\text{s}$ window or OD signal within a $\pm 0.5 \mu\text{s}$ window of a TPC S1 is removed to mitigate γ ray backgrounds. In addition, any event with an OD pulse $> 200 \text{ keV}$ within a $1200 \mu\text{s}$ window after the TPC S1 is also removed to mitigate neutron capture on hydrogen or gadolinium in the OD. The returning γ ray from an OD capture process are further removed by tagging large skin pulses.

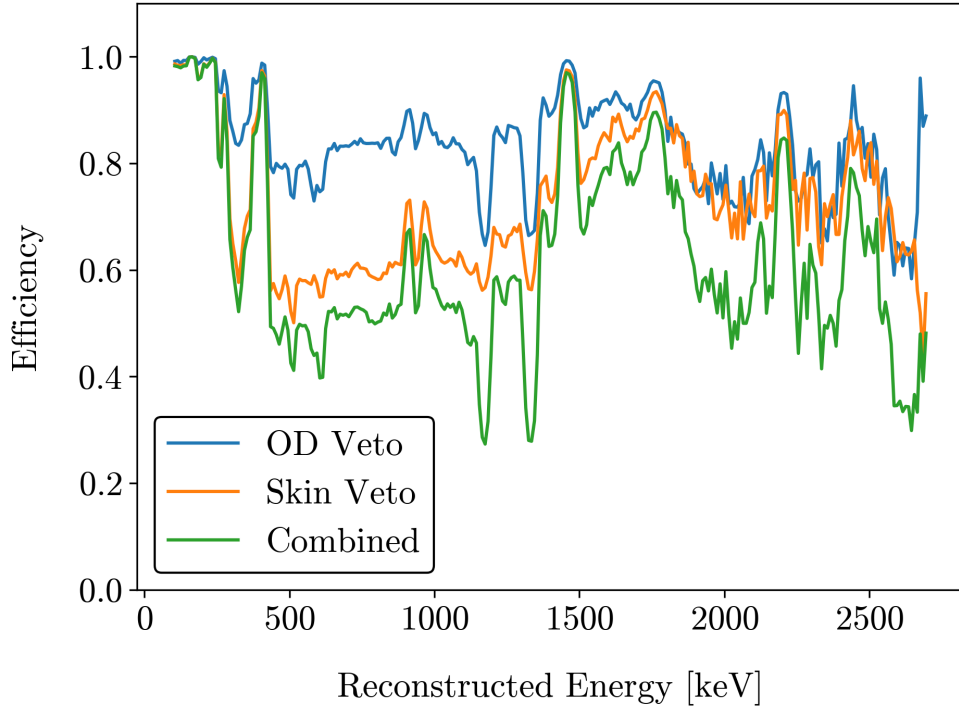


Figure 5.2: The skin and OD veto efficiency. The combined efficiency represents fraction of events that survive both the skin and OD veto cuts.

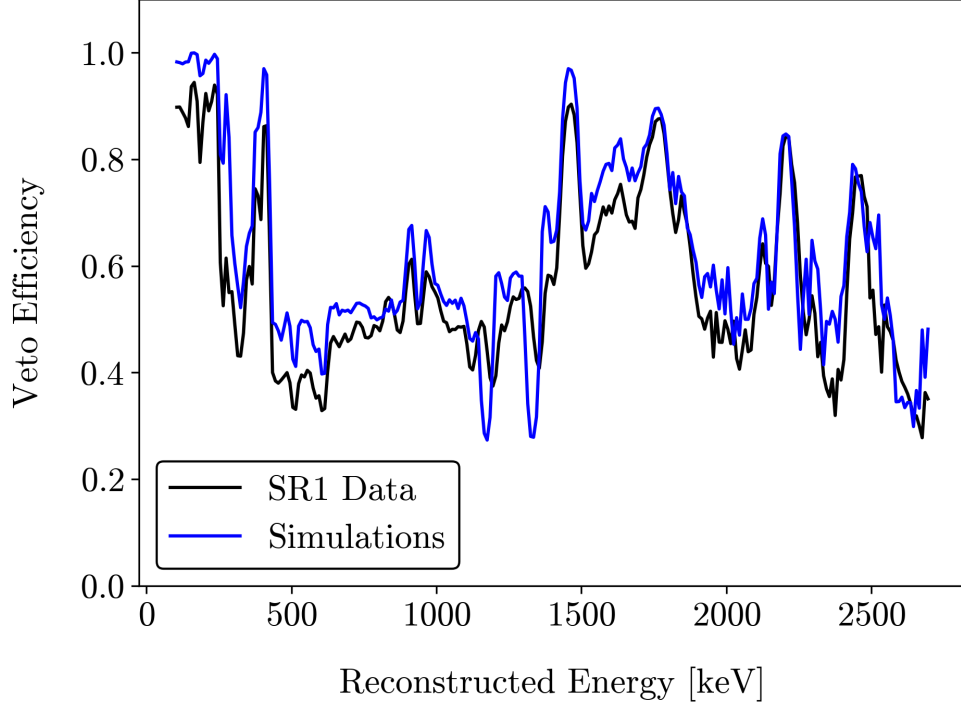


Figure 5.3: Comparison of broad-spectrum response of simulations and SR1 data to vetoes. The overall spectral shape agree well between simulations and SR1 data. Deviations are most noticeable at known γ peaks, which are heavily impacted by the normalisation of corresponding components in the Poisson-sampled dataset.

For this analysis, the veto “efficiency” takes the unusual definition as the fraction of events that survive the veto cuts. Ideally, the efficiency of Skin and OD vetos in simulation and SR1 should be compared with an external broad-spectrum ER calibration source, such as ^{228}Th . However, due to the demonstrative nature of SR1 and the main science target of the WIMP search, such a calibration was not scheduled for SR1. Instead, the ^{228}Th calibrations took place after SR1, with some different tuning to analysis packages that resembles detector conditions in later science runs. For the purpose of comparing broad-spectrum response of simulation and data to the vetoes, the same Poisson-sampled simulation dataset is used to check the overall agreement. The skin and OD veto efficiencies are shown separately in Figure 5.2, together with a combined veto efficiency curve. The response is expected to be heavily impacted by the relative composition of radioactive sources in the sampled dataset, especially γ ray backgrounds from detector components. Taking this into account, an overall

good agreement is demonstrated in Figure 5.3, providing sufficient confidence to include the cuts in the analysis.

FV and ROI

The FV and ROI optimisation described in the sensitivity projection analysis optimises the $S/\sqrt{B}$ ratio for a given background-dominated dataset. This analysis repeats the same optimisation procedure with the SR1 dataset as background and the corrected $n = 1$ energy spectrum as the signal. It is assumed that given the $T_{1/2} > 4.3 \times 10^{24}$ yr lower limit on the halflife of the $n = 1$ mode [38], the accumulated live time of SR1 data taking renders a background-dominated dataset that is suitable for FV and ROI optimisation.

As described previously, the optimisation procedure involves an initial estimate of ROI and FV, followed by scanning over parameters in the vicinity of the initial estimates. The optimal FV parameters along with the relative $S/\sqrt{B}$ value within a given scanned ROI window are recorded, which are then compared to reach a global optimal set of FV and ROI parameters. For the SR1 data, this procedure results in an optimal ROI and FV with the relevant parameters listed in Table. 5.1. Considering that several background sources have peaks outside the suggested ROI, it was decided to disregard the optimal ROI constraint and use the entire energy range for this search, which should result in better fitting of the background model. It is worth noting that the optimal FV parameters differ significantly in the radial direction from that assumed in the sensitivity projection. This results in a smaller fiducial mass of ~ 3.6 t in comparison to the ~ 4.5 t used previously. Much of this is due to the higher-than-expected background rates from detector components in the radial direction of the detector, which will be addressed later in the analysis.

Table 5.1: Summary of the optimised FV and ROI parameters for SR1 $0\nu\beta\beta\phi$ search.

Spectral Index	$\tilde{E}_{min}$ (keV)	$\tilde{E}_{min}$ (keV)	$\tilde{r}$ (cm)	$\tilde{z}_{min}$ (cm)	$\tilde{z}_{max}$ (cm)	Mass (kg)
$n = 1$	1800	2400	58.4	13.0	130.6	3621

5.1.3 ^{136}Xe Exposure after $0\nu\beta\beta\phi$ Search Cuts

The combination of all previously described cuts has an impact on the total equivalent live time of the dataset. Since the set of analysis cuts is different to those used in the SR1 WIMP search, the total remaining live time needs to be calculated separately. Over the calendar span of SR1, taking into account the $\sim 3\%$ live time reduction by exclusion periods, the total run-time recorded from the run control system is 99.6 live days. The OD veto further introduces a 5% down-time to the DAQ. None of the other cuts has a significant impact on the accumulated live time of the dataset. Therefore, the final live time remains is 94.9 live days. This is significantly longer than the 60 live days reported in the LZ WIMP result and will be quoted for the remainder of the analysis.

Another factor that may impact the total ^{136}Xe exposure is its isotopic abundance in the delivered LXe batches. Some anomalous spectroscopy measurements within the LZ collaboration have shown potential signs of minor depletion in ^{136}Xe that deviates from its natural abundance, although this is a small effect yet to be confirmed with independent assays. Since then, samples of LZ Xe have been sent to third-party laboratories for verification. The preliminary result shows that the LZ Xe sample agrees with the isotopic abundance of the lab sample at a level of tens of ppm, confirming that the anomalous measurement is most likely due to systematic uncertainties of the spectrometer. Further independent measurements are planned to verify this result. For the remainder of this analysis, the LXe in the LZ detector is assumed to have natural abundance with no additional systematic uncertainty .

The optimised FV also limits the fiducial mass of LXe utilised for this analysis. Given that the average LXe temperature within the LZ TPC and the literature value of LXe density at 2.87 g/cm^3 [124], the fiducial mass is computed to be 3621 kg, as stated in Table. 5.1. Combined with the impact of analysis cuts on live time, the SR1 data that pass all analysis cuts yields a ^{136}Xe exposure of 83.4 kg·yr. In comparison, the full EXO-200 dataset used to set the most stringent limit of $0\nu\beta\beta\phi$ consists of a ^{136}Xe exposure of 234.1 kg·yr [38]. Due to the difference in exposure to the signal source, we do not expect this analysis to produce

a leading result. Rather, it serves as a demonstration of LZ’s ability to search for $0\nu\beta\beta\phi$ signals, as well as setting the basis framework for future analyses.

5.2 Energy Resolution

Several radioisotopes have γ lines in the vicinity of the $Q_{\beta\beta}$ value of ^{136}Xe at 2458 keV. These include the ^{208}Tl line at 2614 keV and the ^{214}Bi lines at 2119 keV, 2204 keV and 2448 keV. Typical $0\nu\beta\beta$ analyses put great emphasis on improving the energy resolution of the detector, aiming at differentiating the signal peak at $Q_{\beta\beta}$ from the background γ lines. In contrast, the $0\nu\beta\beta\phi$ signal is broad-spectrum in nature, meaning that individual background γ lines are not usually separable from the signal energy spectrum. Therefore, the background rejection capability of a $0\nu\beta\beta\phi$ search does not benefit greatly from a better energy resolution. However, from the perspective of building the background model, a better energy resolution improves the quality of fitting of normalisation factors for individual background components. It is also important to ensure the simulation has the same energy resolution as the real data, such that the two can be better compared at the PLR stage.

Recently, an improved approach to correct for non-uniformity of the light collected by the PMT arrays has been conducted by LZ collaborators [1]. The approach demonstrated the ability to reach a state-of-the-art energy resolution of $0.67\% \pm 0.01\%$ at 2614 keV with SR1 measurements. This unprecedented resolution for any LXe TPC is significantly better than LZ’s previous 1% energy resolution estimate, enabling the sensitivity projection for the $0\nu\beta\beta$ decay to improve from 1.08×10^{26} years to 1.18×10^{26} years.

The caveat of directly quoting this improved energy resolution is that the value was obtained with a different set of analysis cuts in a different fiducial volume, both of which can affect the energy resolution in a non-trivial manner. Therefore, a re-evaluation of the energy resolution with the $0\nu\beta\beta\phi$ search cuts is necessary. The analysis follows the framework described in Ref. [1], adapted to $0\nu\beta\beta\phi$ analysis where necessary. The approach focuses on the correction factor C_2 for the S2 signal, which is a position dependent quantity and is usually normalised

to some fixed reference points for convenience:

$$C_2(x, y, z) = \frac{\langle S2(x_{ref}, y_{ref}, z_{ref}) \rangle}{\langle S2(x, y, z) \rangle}, \quad (5.1)$$

where the angular brackets denote averaging over the dataset. A similar relationship also applies to the S1 correction factor $C_1(x, y, z)$, and the corrected signals $S1c = S1 \cdot C_1(x, y, z)$ and $S2c = S2 \cdot C_2(x, y, z)$ are used in the standard energy reconstruction formula Eq. 2.7. A 3D map of $C_1(x, y, z)$ can be obtained from the measured S1 signals of α emissions in the $^{222}\text{Rn} \rightarrow ^{218}\text{Po}$ decay. On the other hand, the S2 correction factor can be written as a product of position-dependent components:

$$C_2 = C_{lc}(x, y) \cdot C_{ext}(x, y) \cdot C_{elt}(z), \quad (5.2)$$

where C_{lc} is the light collection correction, C_{ext} corrects for charge extraction efficiency, and C_{elt} is the electron lifetime correction. Out of the three components, the C_{elt} is the simplest to calculate as it only depends on a single direction. On the other hand, both C_{ext} and C_{lc} has dependence on x and y , with additional complication of changing operational PMTs affecting C_{lc} . The essence of the approach is to address the problem with C_{lc} by introducing a light response function (LRF), $\lambda_i(x, y)$, for each PMT. This is defined as the fraction of photons detectable by the PMT from isotropic emission at a given position (x, y) . Within this setup, the best estimate of total amount of produced photons, N , has the following relationship with the photons detected by individual PMTs, n_i :

$$\sum_i n_i = N \sum_i \lambda_i(x, y). \quad (5.3)$$

Given that $\langle S2 \rangle = \langle \sum_i n_i \rangle$, the expression of C_{lc} can be written in terms of LRFs:

$$C_{lc} = \frac{\langle S2(x_{ref}, y_{ref}) \rangle}{S2(x, y)} = \frac{\sum_i \lambda_i(x_{ref}, y_{ref})}{\sum_i \lambda_i(x, y)}. \quad (5.4)$$

The detailed parameterisation and computation of the LRFs is beyond the scope of this analysis and can be found in Ref. [1] and the references therein. For the purpose of this analysis, a readily produced LRF map of the PMTs from within the LZ collaboration is used. Energy reconstruction is then performed with $g_1 = 0.1072$ and $g_2^{bot} = 14.51$ as obtained with the Doke plot method (by fitting a straight line to measurements of $S1c/E$

versus $S2c/E$ and obtaining g_1 and g_2 values at line intercepts with the axes [60]), slightly different to the reference values quoted in the SR1 WIMP search result. The relevant γ lines and their corresponding energy values are illustrated in Figure 5.4, along with the binned energy spectrum of SR1 data that passed the analysis cuts.

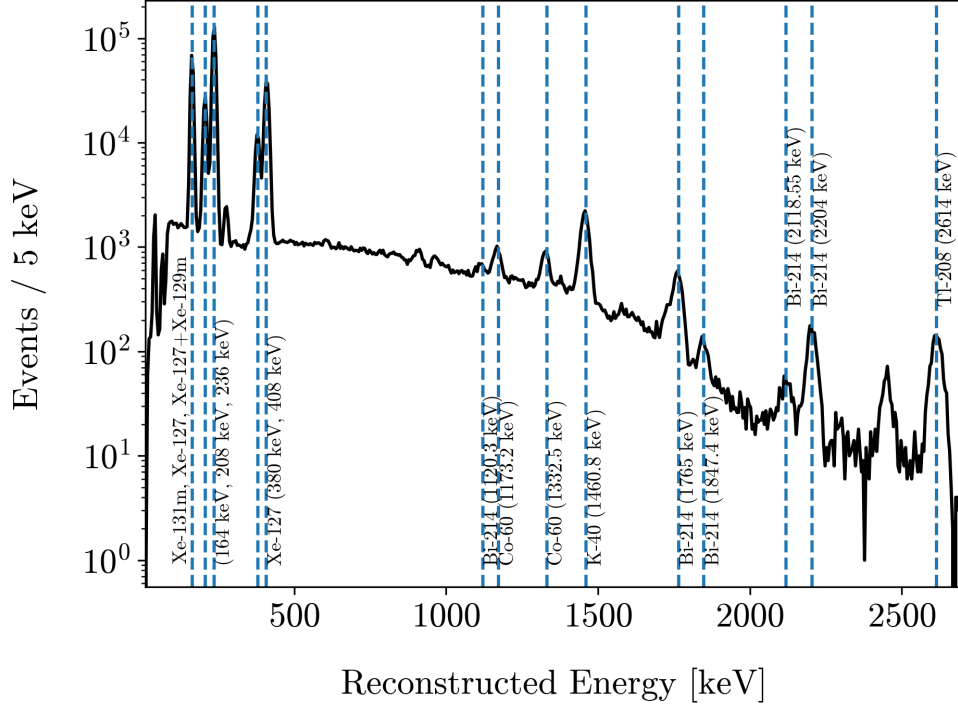


Figure 5.4: The included γ lines for the energy resolution analysis. The true energy values are taken from [112]. The energy spectrum represents SR1 data that pass the $0\nu\beta\beta\phi$ search cuts.

For each γ line, a Gaussian function on top of a linear background is used to fit the peak in data. The energy resolution σ/μ is then obtained from the Gaussian mean and standard deviation. Figure 5.5 shows the obtained resolution values plotted against the corresponding γ line, together with a curve of best-fit that follows the inverse square-root dependence of resolution on energy. The energy resolution is found to be $(0.68 \pm 0.02)\%$ at 2614 keV and a weighted fit of the energy resolution curve is obtained, both of which are in good agreement with the values in the original analysis. Since the simulation has an intrinsic energy resolution tuned to match the 0.67% value at 2614 keV, no further Gaussian smearing is required to

degrade the energy resolution of simulation to real data. The energy spectra of simulated radioactive sources can now be grouped together and directly compare with the energy spectrum of SR1 data.

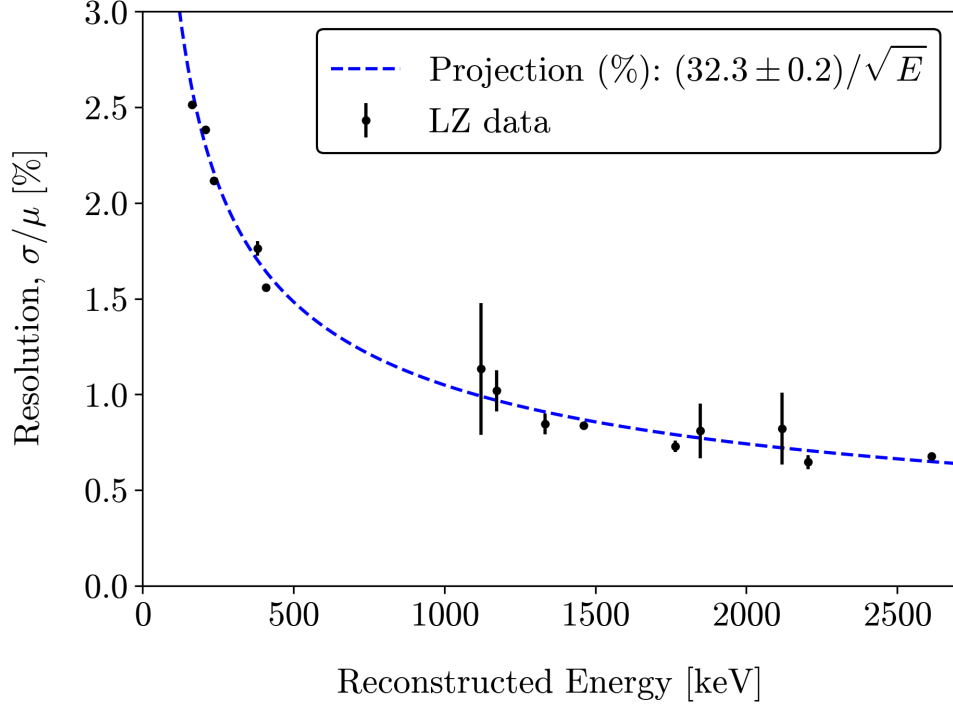


Figure 5.5: Measured energy resolution as a function of the reconstructed energy. The dashed line represents a fitted energy resolution curve.

5.3 Background Model

Analyses in the previous chapters, especially the sensitivity projection, assume a background model that is in steady-state equilibrium. However, several transient components are present in the SR1 dataset and are taken into account by the SR1 WIMP background model [2]. The most notable components of this type are activated xenon radioisotopes, induced by cosmic rays while the xenon is stored above ground and transported to experimental site. The isotopes of consideration include ^{127}Xe , ^{129m}Xe , ^{131}Xe and ^{131m}Xe . As explained previously, the relatively short time separation between the last xenon delivery and the start of SR1 data taking leads to a considerable amount of radioisotopes to be prevalent during SR1.

In addition, neutron calibrations before the science run can also induce xenon activation, contributing further to the prevalent radioisotopes.

Since the long-term contribution of xenon activation to the backgrounds is negligible due to suppression of atmospheric particle fluxes by the rock overburden, the activated xenon isotopes are not included in the background model of $0\nu\beta\beta\phi$ search. In this analysis that compares the background model with the SR1 dataset, the region of energy < 500 keV that is dominated by the decay of activated xenon isotopes is excluded. The benefit of this approach is to omit any time-varying rate of the transient activated xenon components and simplifies the background model. It should help with the convergence of global fitting of the background model by reducing the parameter space to scan through. This comes at a cost of missing signal strength from events within the excluded energy region. For the $n = 1$ mode, only $\sim 1.2\%$ of the signal is in the excluded $0 - 500$ keV region.

With the energy < 500 keV region excluded from comparison, the radioactive sources included in the background model remain the same as those for the sensitivity projection. As before, these sources can be broadly grouped into three categories: internal sources, detector components and cavern rock. For each source, all the $0\nu\beta\beta\phi$ search analysis cuts are applied to its corresponding high-statistics simulations. The energy spectrum of the source is then obtained from energy reconstruction of the simulated events that pass the cuts. A caveat to note is that one may not reuse the energy spectra previously obtained for sensitivity projection and apply a scaling factor. While this works well for internal sources and saves computation power, the spectral shape of any external source (detector components and cavern rock) is highly dependent on the FV due to varying γ attenuation coefficient at different energies. As such, the energy spectra need to be regenerated whenever there is a significant change in the FV.

The generated spectral shape of each source is representative of the $0\nu\beta\beta\phi$ FV, but is subject to normalisation to reflect the activity and uncertainty under SR1 conditions. Bias mitigation also needs to be taken into account, whereby the activity determination should be

performed with calibration data or sideband volumes where possible. The following sections describe the details of activity and uncertainty determination of each radioactive source in the background model. The approach generally follows the comprehensive background determination analysis [2] for the SR1 WIMP search result, with adaptations to the $0\nu\beta\beta\phi$ search where necessary. These activity and uncertainty values are utilised as initial estimates of parameters for a refitting during the PLR analysis.

5.3.1 Internal Sources

Similar to those in the sensitivity projection analysis, the internal sources considered in the background model remain to be the following:

- $^{136}\text{Xe} - 2\nu\beta\beta$
- $^{85}\text{Kr} - \beta$ decay
- $^{212}\text{Pb} - \beta$ decay
- $^{214}\text{Pb} - \beta$ decay
- Solar ν – dominated by the pp -chain, followed by small contributions from ^7Be and the CNO cycle.

Most of the sources in the above list are uniformly distributed in the active LXe. The activity of such a source in a unit volume of LXe is not affected by the selection of analysis cuts, for which results from the WIMP search are directly quoted without reanalysis. The only exception to this assumption is ^{214}Pb , which has a non-uniform spatial distribution due to ion drifting as shown in the previous chapter. This effect is accounted for by introducing a correction factor that represents the ratio of ^{214}Pb events in the $0\nu\beta\beta\phi$ search FV and the SR1 WIMP FV. The correction factor is obtained from the previously demonstrated toy Monte Carlo simulation of ion drifts, with a value of 0.65.

Determination of each of the values is carried outside the $0\nu\beta\beta\phi$ search region, satisfying the requirement of bias mitigation. The ^{85}Kr rate estimate is informed from its natural

abundance and an *in situ* mass spectroscopy measurement of ^{nat}Kr concentration at 144 ± 22 ppq in LZ xenon samples. The ^{136}Xe $2\nu\beta\beta$ rate is estimated to be $4.14 \pm 0.12 \mu\text{Bq}$, determined by its measured half-life [3]. Both ^{212}Pb and ^{214}Pb rates are determined by fitting the peaks of their parent isotopes in the high-energy alpha region ($> 3 \text{ MeV}$), which is outside the $0\nu\beta\beta\phi$ energy range. The estimated rates are calculated to be $0.137 \pm 0.019 \mu\text{Bq/kg}$ and $3.14 \pm 0.22 \mu\text{Bq/kg}$, respectively. And the solar ν contribution to the background is calculated based on relevant measurements [125–127].

5.3.2 Cavern Rock

The normalisation factors of cavern rock γ rays are estimated from rate measurements in the comprehensive SR1 WIMP background analysis, followed by corrections to detector response in the $0\nu\beta\beta\phi$ FV. The rate measurements started with setting the ^{232}Th , ^{238}U and ^{40}K activity of simulated rock shell of the Davis Cavern to previously measured values [113]. The component energy spectra are then fitted to the measured data during commissioning phase of the detector.

The commissioning data were obtained under the detector condition with gaseous xenon target and empty OD and water tank. Removal of external shielding meant that the event rate was heavily dominated by cavern γ rays. Also, the absence of drift and extraction field results in S1-only signals, for which variations in the top-bottom asymmetry (TBA) is used to correct for light collection efficiencies. The corrected S1 signals are then used for energy reconstruction to obtain the energy spectrum. Since the entire energy reconstruction and fitting process is performed under different detector condition to the SR1 data, the obtained normalisation factors are bias-mitigated for the purpose of $0\nu\beta\beta\phi$ search. The normalisation factors are then applied to energy PDFs of high-statistics simulations that pass the analysis cuts, ensuring the scaled PDFs are representative of the SR1 dataset.

5.3.3 Detector Components

Amongst the three categories of radioactive backgrounds, the contribution from detector components is perhaps the most difficult to deal with. Not only is it highly dependent on the FV of choice, the large number of individual components and their geometrical allocation all need to be simulated with proper assignment of activity and uncertainty. The situation is further complicated by the fact that even for the same decay chain, differing trajectories to reach the LXe target render variation in the relative spectral shape of simulation outputs for different components. The procedure to estimate background activities and uncertainties from detector components was developed and carried out by LZ collaborators for the SR1 WIMP background determination [2]. This analysis follows the same procedure, with adaptations to the $0\nu\beta\beta\phi$ search where necessary.

Instead of considering every single simulated component separately in the fitting, sources are rearranged into groups for which the scaling factors are fitted collectively. There are two requirements for components to be assigned the same group: they should belong to the same decay chain, and their spectral shapes are deemed similar enough. A Kolmogorov-Smirnov (KS) test statistic and an upper threshold of 0.1 is set for grouping. In general, sources that are in physical proximity in the detector are likely to satisfy this requirement.

Even with the significantly reduced number of components to fit, a simultaneous optimisation is still beyond the available computational resources. The fitting is therefore carried out successively by selecting sub-volumes within the TPC, where certain components are expected to dominate the backgrounds due to the geometric location of the detector components. The sub-volumes considered are top, side and bottom volumes, as illustrated in Figure 5.6. It is evident that the sub-volumes have very little overlap with the $0\nu\beta\beta\phi$ FV, and component activity determined from these sub-volumes are bias-mitigated for the final $0\nu\beta\beta\phi$ search.

A relatively loose 1% prominence requirement is set for the $0\nu\beta\beta\phi$ analysis. Any compo-

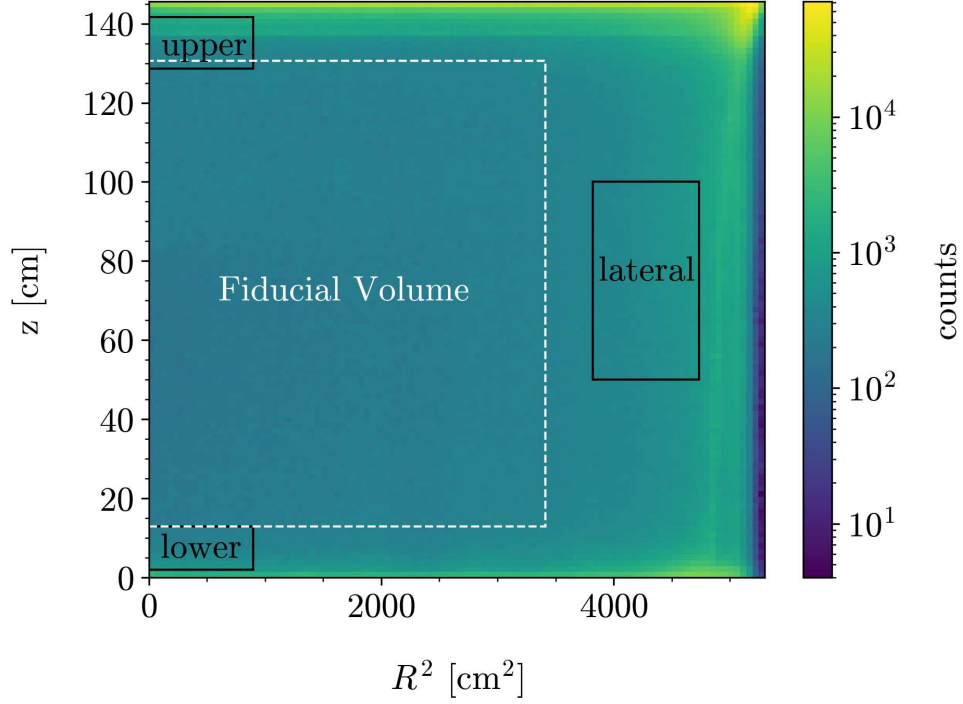


Figure 5.6: Sub-volumes for successive fitting of γ ray backgrounds from detector components. The relative locations of the sub-volumes and the $0\nu\beta\beta\phi$ fiducial volume within the TPC are shown.

ment that has higher contribution than this threshold and satisfies the spectral similarity requirement are deemed prominent. Other components are considered as sub-dominant and therefore have fixed normalisations during the fit. The fitted parameters of a given sub-volume are then used as constraints for the respective components in successive fits.

The fitting procedure starts with setting internal components to their respective activity. An energy range of 1000 – 2700 keV is then used to eliminate contributions from internal radioactive sources, whilst also capturing the ^{208}Tl γ peak at 2614 keV. Fitting is then performed in the sub-volumes, starting from the side, then to the bottom and finishing at the top volume. The fitted scaling factor of each decay chain within the sub-volumes are illustrated in Figure 5.7.

After constraining the scaling factors and uncertainties of each component, their summed

rates in the sub-volumes as well as the total contributions to the $0\nu\beta\beta\phi$ FV are computed as listed in Table 5.2. For each decay chain, the summed high-statistics energy PDFs of detector components are then scaled accordingly. This ensures the energy PDFs that enter the PLR stage have spectral shapes and normalisations that are representative of the $0\nu\beta\beta\phi$ FV.

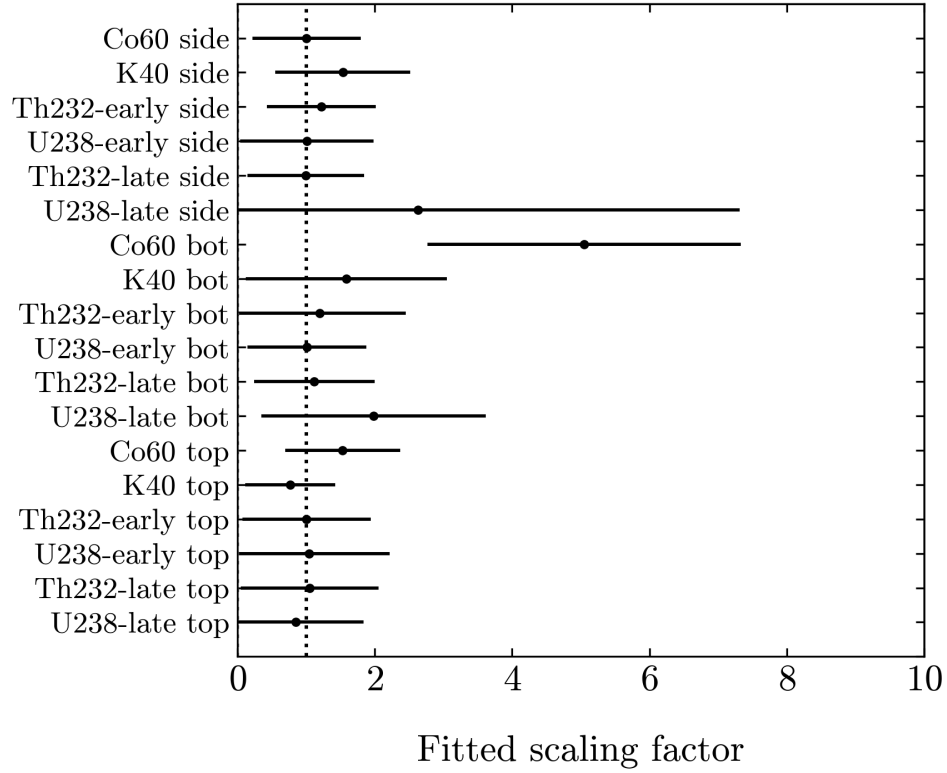


Figure 5.7: Scaling factors for radioactive sources in their respective sub-volumes. The dotted vertical line represents the expected rates from screening assay [68].

Table 5.2: Summed activities of sources in the FV fit.

Isotope/Chain	Region	Screening estimate [Bq]	Best fit [Bq]
^{60}Co	Top	3.04 ± 0.30	3.63 ± 2.60
	Side	0.63 ± 0.06	0.63 ± 0.54
	Bottom	0.46 ± 0.05	2.67 ± 1.18
	Total	4.12 ± 0.31	6.93 ± 2.91
^{40}K	Top	7.22 ± 0.72	4.88 ± 6.16
	Side	2.56 ± 0.26	4.19 ± 2.78
	Bottom	3.97 ± 0.40	6.41 ± 5.96
	Total	13.74 ± 0.86	15.48 ± 9.01
$^{232}\text{Th-early}$	Top	0.85 ± 0.08	1.05 ± 0.98
	Side	0.20 ± 0.02	0.23 ± 0.17
	Bottom	0.10 ± 0.01	0.13 ± 0.16
	Total	1.14 ± 0.09	1.41 ± 1.01
$^{232}\text{Th-late}$	Top	0.90 ± 0.09	0.95 ± 0.92
	Side	0.36 ± 0.04	0.37 ± 0.35
	Bottom	0.11 ± 0.01	0.14 ± 0.17
	Total	1.37 ± 0.10	1.45 ± 1.00
$^{238}\text{U-early}$	Top	4.84 ± 0.48	4.95 ± 5.29
	Side	0.73 ± 0.07	0.73 ± 0.71
	Bottom	1.21 ± 0.12	1.21 ± 1.17
	Total	6.78 ± 0.50	6.90 ± 5.46
$^{238}\text{U-late}$	Top	0.97 ± 0.10	0.91 ± 0.66
	Side	0.10 ± 0.01	0.26 ± 0.45
	Bottom	0.67 ± 0.07	1.52 ± 1.28
	Total	1.75 ± 0.12	2.68 ± 1.51

5.3.4 The Complete Background Model

With all components of the background model constrained, the rescaled energy PDFs of individual components are assembled together to reach the complete background model as illustrated in Figure 5.8. The summed energy spectrum of the complete background model is then compared with SR1 data in the energy range of 500 – 2700 keV, with percentage deviations from data shown in Figure 5.9. It is evident that the deviations are generally well controlled within 50%, except for the > 2000 keV region where larger deviations are observed. This is partly due to the relatively low statistics of high-energy events in data, as well as the bias-mitigating approach of fitting in sideband volumes rather than on data itself. Since the likelihood computation is weighted by bin height, the deviation of model from data in the high-energy region should not pose serious problem to the PLR analysis. One should also note that the model should not be used directly for statistical inference. Instead, it serves as an input for the global fitting prior to the PLR analysis.

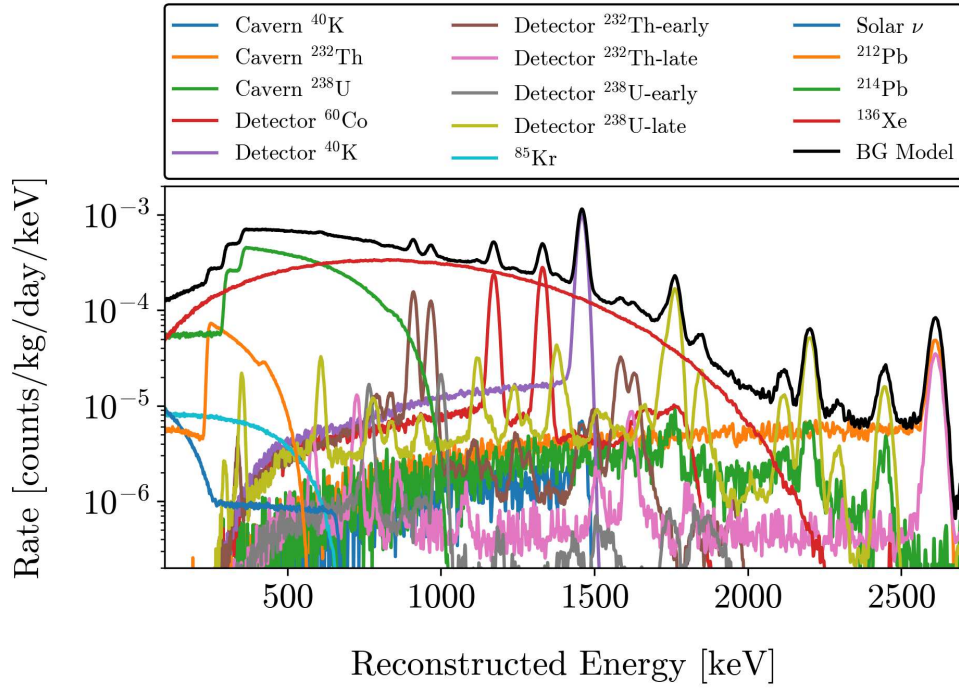


Figure 5.8: Energy spectra of the complete background model for SR1 $0\nu\beta\beta\phi$ search. Each component is scaled to match the measured activity in the fiducial volume.

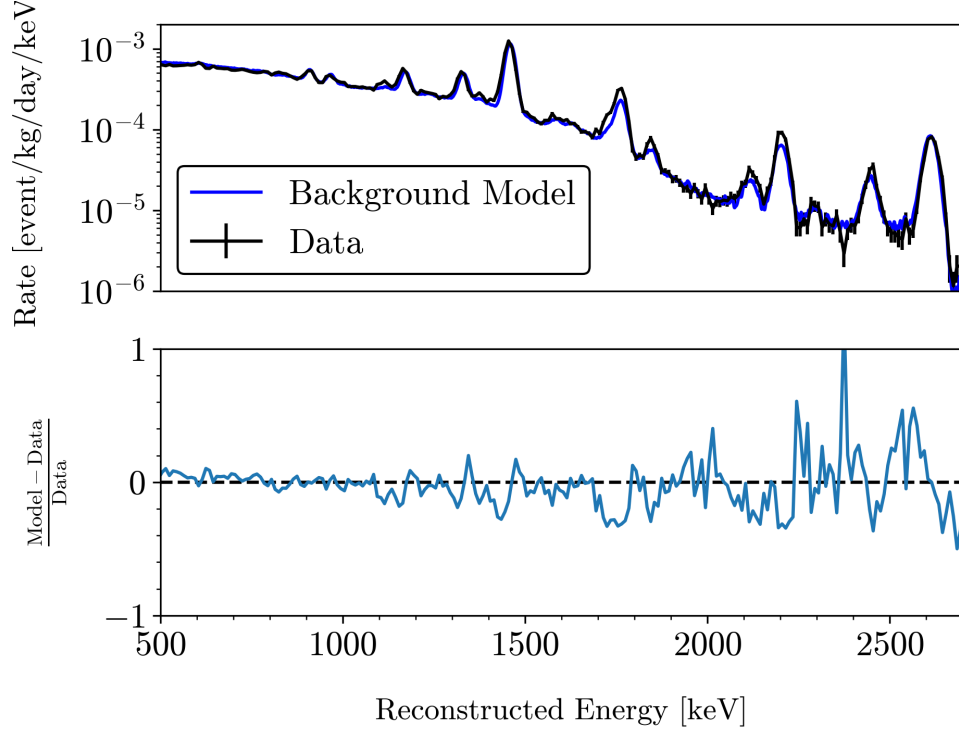


Figure 5.9: Comparison of the complete background model with SR1 data. The error bars represent statistical uncertainties in SR1 data, although too small to be visible at lower reconstructed energies in the figure due to large statistics of events.

5.4 $2\nu\beta\beta$ Validation

An ideal benchmark to demonstrate the validity of the background model is to showcase that a global fitting recovers the correct activity for other background components. The ^{136}Xe $2\nu\beta\beta$ spectrum has an accurately measured half-life and natural abundance, making it a perfect candidate for this purpose. The goal is to constrain the global fitting only to the high-energy region of the spectrum, where sideband fitting of detector components shows significant deviation from data. Provided that the global fitting result of ^{136}Xe $2\nu\beta\beta$ agrees with expectation, the model deviations are acceptable and a global fitting with the full energy range can be performed for further PLR analysis.

The fitting is performed in the energy range of 1900 – 2700 keV, within which a total of 5437

events are observed in the SR1 dataset. Several background sources have negligible activity within this energy range, including ^{40}K and ^{232}Th -early in detector components, ^{40}K in cavern rock, and all internal sources except for ^{136}Xe . Contributions from these sources are excluded from the fitting. It is expected that ^{136}Xe $2\nu\beta\beta$ decays account for $\sim 10\%$ of events in the simplified background model, a significant yet not dominant proportion. This gives enough flexibility for each component to vary, without being overwhelmingly dominated by a single source and leading to vanishing gradient when computing likelihoods.

Table 5.3: Summed activities of sources in the combined fit for $2\nu\beta\beta$ validation. The uncertainties in the expected events are from individual component determination and those in the fit results are the errors on the best fit values.

Group	Source	Expected Events	Fit Results
Detector Components	^{60}Co	8.6 ± 3.6	6.1 ± 3.6
	^{232}Th -early	18.3 ± 13.2	49.3 ± 12.2
	^{232}Th -late	646.0 ± 445.8	824.5 ± 66.5
	^{238}U -late	1303.2 ± 729.8	2122.0 ± 68.2
Cavern Rock	^{232}Th	2025.3 ± 202.5	1663.6 ± 98.8
	^{238}U	408.7 ± 110.4	226.9 ± 70.8
Internal Sources	^{136}Xe	562.5 ± 28.1	536.9 ± 57.9
Total		4972.5 ± 886.3	5429.3 ± 165.4

Table 5.3 shows the expected number of events and the fit result for each source. The uncertainties in the expected rate account for both statistical and systematic ones. The statistical uncertainties are the inferred values from the determination procedure of each component as previously described. On the other hand, systematic uncertainties mainly come from the ^{136}Xe exposure estimation and event reconstruction in the SR1 dataset. It is estimated that the total LXe mass within the FV has a 3.6% systematic uncertainty due to spatial resolution of the detector at this early stage of analysis. In addition, a 1% systematic uncertainty is attributed to the total live time and a further 2% to the SS event reconstruction. The total systematic error is thus estimated to be about 4.2%, which is significant for ^{136}Xe ,

but subdominant for external sources given their large statistical uncertainties in the narrow energy range of 1900 – 2700 keV. The uncertainties of all sources are then included in the Gaussian constraint terms of the likelihood function Eq. 3.7.

The global fitting is performed essentially unconstrained, where the activity of each source can vary between zero and ten times its expected value. Some of the sources have fit results that are different from expectations but none of them deviate by more than two standard deviations. The key takeaway is the decent agreement between fit result and expected number of ^{136}Xe $2\nu\beta\beta$ events. The best fit value of 536.9 ± 57.9 events from profile likelihood scan incorporates the 4.2% systematic error mentioned above and a 9.9% statistical uncertainty. In this case, the total relative uncertainty is dominated by statistical uncertainties because of the limited number of events in the validation energy range. If converting to half-life measurements, the fit result corresponds to a measured half-life of $T_{1/2} = 2.25 \pm 0.22 \times 10^{21}$ years. This is indeed in good agreement with the literature value of $T_{1/2} = 2.165 \pm 0.016(\text{stat.}) \pm 0.059(\text{sys.}) \times 10^{21}$ years [3]. Moreover, it shows the level of deviations of the background model from data still allows for correct global fitting of other components, validating the usage of the model at its current state for further analysis.

5.5 SR1 $0\nu\beta\beta\phi$ Search Result

Statistical inference on the half-life of the $n = 1$ mode of $0\nu\beta\beta\phi$ is performed over the reconstructed energy observable space. A one-sided binned profile likelihood test statistic at 90% confidence level is used. The expected rates of the background components are allowed to vary during refitting to achieve the maximum likelihoods, and the uncertainties of each component are included as nuisance parameters to constrain the combined fit.

The expected number of events from sideband and calibration constraints, and the fit result are shown in Table 5.4. Uncertainties are estimated with the same procedure as to the ^{136}Xe $2\nu\beta\beta$ validation analysis, and the expected rate in Table 5.4 account for both statistical and systematic errors. The only difference between this and Table 5.3 is that it utilises a

wider energy range of 500 – 2700 keV and includes all background sources of interest. The fit results of nearly all components agree with expectation, except for the cavern rock that fall slightly below the expected range. This is not surprising as γ flux from the cavern rock is extremely difficult to constrain accurately, due to the huge suppression provided by the water shield. Since the contribution of the cavern components are subdominant in the model, the slight deviation has very little impact.

Table 5.4: Summed activities of sources in the combined fit for $0\nu\beta\beta\phi$ search. The uncertainties in the expected events is from individual component determination and those in the fit results are the errors on the best fit values.

Group	Source	Expected Events	Fit Results
Detector Components	^{60}Co	8142 ± 3419	8571 ± 190
	^{40}K	14588 ± 8461	16011 ± 166
	^{232}Th -early	4680 ± 3370	3816 ± 211
	^{232}Th -late	1179 ± 813	1478 ± 124
	^{238}U -early	542 ± 428	354 ± 167
	^{238}U -late	7229 ± 4048	12102 ± 198
Cavern Rock	^{40}K	431 ± 65	295 ± 64
	^{232}Th	3554 ± 355	2877 ± 192
	^{238}U	1488 ± 402	417 ± 231
Internal Sources	^{136}Xe	100306 ± 5015	105151 ± 675
	^{85}Kr	97 ± 15	107 ± 15
	^{212}Pb	67 ± 9	75 ± 9
	^{214}Pb	30984 ± 9295	26426 ± 342
	Solar ν	49 ± 1	48 ± 1
Total		173337 ± 14957	177728 ± 926

PLR inference shows that the SR1 data agree with the background-only hypothesis with a p-value of 0.96. At 90% confidence level, the data exclude an upper limit of 1125 signal events. Considering the MS branching ratio correction due to bremsstrahlung, and the

exclusion of data below 500 keV, the signal detection efficiency is estimated to be 89.8%. The combined effect of efficiency correction and exclusion limit corresponds to a lower limit of $T_{1/2} > 2.1 \times 10^{23}$ yr for the $n = 1$ mode of $0\nu\beta\beta\phi$ in ^{136}Xe .

This search result is based on the initial science run of LZ, which is an early science run aimed at understanding and optimising the detector performance under stable conditions. The analysis cuts and tools readily available within the collaboration at the time of writing are mostly optimised for WIMP direct detection, while the collaboration is carrying out ongoing work to cater for other scientific objectives. Nevertheless, with the available analysis framework and some development, the necessary steps required to obtain a $0\nu\beta\beta\phi$ search result have been demonstrated. The lower limit of $T_{1/2} > 2.1 \times 10^{23}$ yr is in relative good agreement with the sensitivity projection, which corresponds to $T_{1/2} > 3.0 \times 10^{23}$ yr after scaling to the same ^{136}Xe exposure as the SR1 dataset. While the result is not yet competitive to the current best limit of 4.3×10^{24} yr [38], the agreement between data and expectation provides solid support to the claim of LZ’s competitiveness in future searches of $0\nu\beta\beta\phi$.

The search result also does not explore the full potential of the SR1 dataset. There are a few limitations at the time of this analysis work, which can be addressed in the near future. For example, only a subset of analysis cuts developed by the LZ collaboration are used for this demonstrative $0\nu\beta\beta\phi$ search, with many more available and optimised for the WIMP search. Examples of such cuts include tagging events originating from electron pile-ups after the tail of an event with large energy deposition, and many more. Understanding the response and re-optimising these analysis cuts for the $0\nu\beta\beta\phi$ search will require significant work, but has the potential to significantly reduce the background events in the selected dataset for PLR inference.

LZ is currently operating and taking data continuously under stable detector conditions. The accumulated data will increase the statistics available for high-energy γ ray events, reducing the uncertainty on the activity of many background sources. While this is unlikely

to bring LZ's capability to search for the $n = 1$ mode close to the current best limit of 4.3×10^{24} yr [38], closing the gap to within an order of magnitude is a reasonable expectation. More importantly, cosmogenic radioisotopes have now decayed away, and the radon veto developed within the LZ collaboration has demonstrated a promising preliminary efficiency. Together with other improvements on background determination, the future background model has great potential to search for $0\nu\beta\beta\phi$ with larger spectral indices, utilising LZ's low energy threshold and optimised background levels in the lower energy region. Within the designed life-time of the detector, it is a perfectly valid expectation for LZ to achieve world-leading results in the field of $0\nu\beta\beta\phi$ searches.

Chapter 6

Conclusions

The work of this thesis has focused on demonstrating the ability and future potential of the LUX-ZEPLIN (LZ) experiment to search for ^{136}Xe $0\nu\beta\beta\phi$ decay process. Chapter 3 discusses the steps of analysis required for a sensitivity study, and the results show that LZ can achieve competitive results within its planned operation lifespan, even comparing to dedicated experiments using enriched xenon. Specific to each spectral index, LZ has an expected sensitivity to exclude $T_{1/2} < 4.75 \times 10^{23}$ yr, $T_{1/2} < 8.36 \times 10^{23}$ yr, $T_{1/2} < 3.40 \times 10^{23}$ yr, and $T_{1/2} < 4.90 \times 10^{22}$ yr at 90% CL for $n = 1, 2, 3, 7$ modes, respectively, after a conservative 500 livedays. Since the detector design is optimised for direct detection of WIMP dark matter, LZ is particularly competitive for $0\nu\beta\beta\phi$ models with higher spectral indices, where the signal energy spectrum skews towards the lower end.

The analysis presented in this thesis has focused in particular on an important background source, ^{214}Pb , which has shown a spatially varying distribution in the TPC, as hoped during detector design but only confirmed now with real data. A novel tagging method based on the multiple-scatter branching ratio has been explored, but the prevalent activated xenon backgrounds in the early dataset means the approach will only be valid for future LZ data. A toy Monte Carlo approach is taken instead to estimate the ^{214}Pb spatial distribution. This then allows one to quantify the impact of ^{214}Pb spatial non-uniformity on LZ's sensitivity to $0\nu\beta\beta\phi$, which turns out to be nearly negligible.

Following the completion of LZ’s initial science run (SR1), Chapter 5 demonstrates a search for the $n = 1$ mode of $0\nu\beta\beta\phi$ in ^{136}Xe with the SR1 dataset. An intermediate step of the analysis involves fitting of the background model, which confirms the literature value of half-life of $2\nu\beta\beta$ decay within experimental error. The search result shows that LZ excludes $T_{1/2} < 2.1 \times 10^{23}$ yr for the $n = 1$ mode of $0\nu\beta\beta\phi$ in ^{136}Xe at 90% CL. This is in good agreement with the expectation from the sensitivity study when scaled to the same ^{136}Xe exposure. The result is a definitive proof that, despite being optimised for direct detection of $\mathcal{O}(\text{keV})$ WIMP interactions, LZ has the versatility to search for other processes such as $0\nu\beta\beta\phi$. The multi-purpose nature of the dual-phase xenon TPC detector technology is especially valuable for future generation experiments.

At the time of writing this thesis, LZ is operating under stable detector conditions and continuously taking data. The accumulated data with sufficiently large ^{136}Xe will allow LZ to produce competitive search results in the near future. With the transient cosmogenic xenon backgrounds decaying away over time, and the larger statistics of high-energy events, the overall high-energy ER background model for the $0\nu\beta\beta\phi$ search is expected to improve. This should enable LZ to utilise its low-background design in the lower end of the energy spectrum and demonstrate advantages in the search of $0\nu\beta\beta\phi$ modes with large spectral indices.

Some exploration projects throughout this PhD journey have not been included in the thesis, but can be potential future areas of improvement for the $0\nu\beta\beta\phi$ search. An example of this is to construct background models with both energy and spatial dependence. This would require large statistics but can help differentiating external backgrounds from internal ones. Another example is to use generative models such as conditional generative adversarial networks (GAN) to generate large statistics of high-energy Monte Carlo simulations based on input conditions. This approach can significantly reduce the monetary and computational burden of future experiments.

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