Enhanced search sensitivity to double beta decay of $^{136}$Xe to excited states with topological signatures

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Abstract: Double beta decay of $^{136}$Xe to excited states of $^{136}$Ba (DBD-ES) is not discovered experimentally yet. The experimental signature of such decays, one or two gamma rays following the beta signals, can be identified more effectively in a gaseous detector with the help of topological signatures. We have investigated key parameters of particle trajectories of DBD-ES with Monte Carlo simulation data of the proposed PandaX-III detector as an example. The background rates can be reduced by about one order of magnitude while keeping more than half of signals with topological analysis. The estimated half-life sensitivity of DBD-ES can be improved by 1.8 times to $4.1 \times 10^{23}$ yr (90% CL). Similarly, the half-life sensitivity of neutrinoless double beta decay of $^{136}$Xe to excited states of $^{136}$Ba can be improved by a factor of 4.8 with topological signatures.

Key words: Neutrino, Double beta decay, Topological signatures, Background suppression, Machine learning

1 Introduction

Double beta decay (DBD) is a rare nuclear process in which two beta decays happen simultaneously in a nucleus [1]. The decay to the ground state of its daughter, which is commonly referred as DBD for short, has been observed in 11 isotopes, including $^{136}$Xe, $^{130}$Te, and $^{76}$Ge. Most of the half-lives are in the range of $10^{19}$ to $10^{24}$ years. Double beta decay to the excited states (DBD-ES), due to the smaller branching ratio and longer half-lives, has only been observed in a couple of isotopes. DBD of $^{136}$Xe to the ground states of $^{136}$Ba was discovered by EXO-200 [2] and then confirmed by KamLAND-Zen [3]. The two collaborations have searched for DBD-ES of $^{136}$Xe with null results so far. If DBD-ES is observed, the comparison between half-lives of DBD and DBD-ES can provide critical input to evaluate the nuclear matrix elements (NME) [4] of the decay and help understanding the rare nuclear process in general.

The hypothetical DBD process without neutrino released, which is called neutrinoless DBD (NLDBD), is of great importance for nuclear and particle physics. NLDBD is a lepton-number-violating process [5] and would also prove the Majorana nature of neutrinos [6]. NLDBD to ground states are actively being searched in different candidate isotopes and the established half-life limits can be as long as $10^{26}$ years. NLDBD to excited states (NLDBD-ES) is also possible but with even longer half-lives compared to the decay to ground states.

The $^{136}$Xe decay to the $0^+_1$ excited state of $^{136}$Ba with energy released of 878.8 keV is the dominate one among all possible (NL)DBD-ES channels. The energies of the subsequent de-excitation $\gamma$ rays are 760.5 keV and 818.5 keV respectively. Hence, we focus our studies on the decay to the $0^+_1$ excited state. In the NLDBD-ES case, two electrons carry away the total energy. While in DBD-ES, the two electron energy spectrum is a continuous one with end point at 878.8 keV.

The de-excitation $\gamma$ ray(s) is essential to enhance the signal over noise ratio in experimental searches. Coincidence between electron-pair and de-excitation $\gamma$ rays can be found in multiple modules of a detector array or different parts of one large monolithic detector. Gaseous detector can measure the detailed energy deposition along particle trajectories and identify the electron-pairs and $\gamma$ rays by the characteristics of trajectories. We argue that the topological analysis on particle tracks can enhance the search sensitivity to (NL)DBD-ES.

We take the proposed PandaX-III [7] detector as an example of high pressure gaseous Time Projection Chamber (TPC) [8] for our studies. PandaX-III aims to build a detector with 140 kg of 90% $^{136}$Xe-enriched xenon to search for double beta decay of $^{136}$Xe in the China Jin-Ping underground Laboratory (CJPL). It will be operated at 10 bar pressure and the active volume is 1.6 m in diameter and 1.2 m in length. Xenon gas will be mixed with approximately 1% Trimethylamine to suppress scintillation light of xenon and diffusion ef-
fect of electron drift \cite{9,10}. Subsequently only ionization signals are read out and amplified with Micromegas module (MM) \cite{11}. The target energy resolution at $Q_{NLDBD} = 2457.8$ keV is $3\%$ Full Width at Maximum (FWHM) \cite{12}.

Figure 1. Illustration of the PandaX-III detector reconstructed in MC simulation. The most prominent features include two outside shielding layers (light green), SS vessel (light blue), and copper pieces (orange-red).

2 Detector simulation with Geant4

Our Monte Carlo simulation is based on the detector geometry of the current conceptual design of PandaX-III experiment \cite{13}. As shown in Figure 1, the detector is enveloped in a Stainless Steel (SS) cylindrical vessel. The thicknesses of the vessel barrel and the end-caps are 1 cm and 1.8 cm respectively. The bottom torispherical cap is welded with the barrel and the top one is connected with the barrel by two flanges. The total SS mass is approximately 2.5 t. The detector is a single ended design with the readout plane on top and the cathode on the bottom. A cylindrical field cage connecting the two parts consists of a 5 cm thick ultra-pure oxygen-free copper is inserted. Two torispherical copper shielding blocks above and below the TPC are also added. The total mass of the copper liner reaches 22.6 t. One layer of lead and one layer of High Density Polyethylene (HDPE) are placed outside the vessel. The thickness of these two shielding layers is 30 cm each.

Figure 2. Work flow of simulation and analysis in six stages, shown in rectangles from top to bottom. In the third stage, detector response, such as gas medium properties and charge readout schemes are added. The blue ovals on the right denote data types transmitted between adjacent stages.

Figure 2 illustrates the complete work flow to simulate and analyze (NL)DBD-ES signals in 6 different stages. In the first stage, energy and angular distribution of emitted particles from (NL)DBD-ES events are generated with the Decay0 package \cite{15}. The simulated signal events are then used for the Geant4 \cite{16} with the geometry described previously. Simulation of background events starts from the second stage. For the PandaX-III detector setup, we simulate background contributions from major sources, including bulk contamination of $^{238}$U and $^{232}$Th in Micromegas, the copper liner, the SS vessel, and the acrylic field cage. For the copper liner, $^{60}$Co and $^{40}$K contaminations are also considered. The contamination levels used in the simulation are shown in Table 1. We also take into account of the
surface radioactivity of Micromegas, which has an upper limit of 45 nBq/cm² and 14 nBq/cm² for $^{238}$U and $^{232}$Th respectively [17].

Large sets of signal and background data are generated and simulated to have enough statistics of training and testing samples in the efficiency studies later. We simulate 10 and 20 million of DBD-ES and NLDBD-ES events respectively. The simulated number of background events from different radioisotopes in different detector components are weighted by contamination levels and mass of the component. For example, $6.52 \times 10^8$ from $^{238}$U chain, $1.74 \times 10^8$ $^{232}$Th chain, $1.74 \times 10^9$ $^{60}$Co, and $2.00 \times 10^{10}$ $^{40}$K events originate from copper liner are simulated. Additionally, we generate $3.48 \times 10^7$ ($1.08 \times 10^7$) $^{238}$U ($^{232}$Th) events from Micromegas and $3.80 \times 10^8$ ($1.24 \times 10^8$) $^{238}$U ($^{232}$Th) events from acrylic. Due to effective shielding of copper liner, the efficiency of γ rays from SS vessel reaching the active volume of the detector is extremely low and the effect of contamination from SS vessel is scaled from that of copper liner by radioactive levels and shielding effects.

| Component | Material          | Activity (µBq/kg) | $^{238}$U | $^{232}$Th | $^{60}$Co | $^{40}$K |
|-----------|-------------------|-------------------|-----------|-----------|-----------|----------|
| Liner     | Copper [18, 19]    | 0.75              | 0.20      | 2         | 23        |
| Field Cage| Acrylic [20]       | 13.68             | 4.48      | -         | -         |
| Vessel    | Stainless Steel [21]| 500               | 320       | -         | -         |
|           |                    |                   |           |           |           |

Table 1. Bulk radioactivities of isotopes for major components considered in the simulation.

The next three stages are implemented in REST [22], a software package developed for simulation and track reconstruction in TPC-based detectors. Details of signal generation, simulation, reconstruction, and analysis in the framework can be found in [22, 23]. Response of TPC, such as electron diffusion and energy smearing, is added in the third stage. Energy deposition is also grouped by the readout strips of Micromegas and the effective coverage of readout plane is taken into account. In the fourth stage, we reconstruct the particles’ tracks with energy and timing information from readout strips. Subsequently, we extract key parameters to characterize reconstructed tracks. One example of track characteristics is blob energy, which describes energy deposition at the end of the trajectory. For an electron traveling in medium, the energy loss per unit volume right before it stops is larger than that along the trajectory due to Bragg peak and more zigzag tracks at the end. The energy loss within a certain spherical volume by the end of the track is called blob energy and the ratio between the smaller blob energy over the larger one is defined as blob ratio or QR for short. QR for the track of two electrons originating from (NL)DBD-ES decays is closer to one compared to that of background events. Figure 3 shows two example tracks from NLDBD-ES and a background event from the $^{238}$U chain. The NLDBD-ES event (left) contains two electrons with a total energy of 878.8 keV (the green track) and one γ ray with 818.5 keV (the red track). One can see the distinct feature of two large blob energies for the dual-electron track. The background event on the right can be seen with one small blob energy at the upper end of the track. Besides QR, other discriminating parameters will be introduced in Section 3 and 4 respectively corresponding to the case of DBD-ES and NLDBD-ES.

![Figure 3. Reconstructed tracks of an example NLDBD-ES event (left) and a background event coming from Micromegas $^{238}$U (right). Only the X-Z projections of the tracks are shown. The total energy of both events are in the range of [1645.3, 1749.3] keV.](image)

Lastly, we classify events into signal or background by the distribution of track parameters with the Toolkit for Multivariate Analysis (TMVA) [25] in the ROOT framework. These backgrounds and signals are equally divided into training and test datasets at random for TMVA classification. TMVA ranks every testing event with a discriminator variable between -1 and 1, which means a background-like and signal-like event respectively. The classification is then compared with MC truth to calculate relevant efficiencies and subsequent significances.

### 3 Double beta decay to $0^+\text{T}$ excited state

For DBD to $0^+\text{T}$ excited state, we define the analysis region of interest (ROI) based on main tracks (MT), the most energetic track in an event. The sum of the energy of the MT in the XZ and YZ planes is called $\text{MTE}$. In the MTE spectra, ROIs [725.7, 789.0] keV and [789.0, 854.6] keV are defined around the two de-excitation γ-rays from $^{238}$U and $^{232}$Th respectively.
peaks at 760.5 keV and 818.5 keV. The range of the ROIs is 2\(\sigma\) from the center but the widths of two connecting sides are shrunk to 1.6\(\sigma\) to avoid overlapping. We define eight additional parameters based on the characteristic of reconstructed tracks, described as follows.

Three global parameters are the total deposited energy (denoted as Energy), the total number of tracks (nTracks), and the track dispersion (\(K\)), the last of which is defined as:

\[
K^{XZ(YZ)} = \sum_{i=1}^{N} E_i \quad \text{for hits} \in S,
\]

where \(E_i\) represents the energy of the \(i\)th hits of an event within a circle \(S\), which is centered at the energy-weighted center of the event on the XZ (YZ) plane. The radius of \(S\) is optimized to be 12.5 mm.

Three more parameters related to MT are the projected MT length at each plane (\(L\)), the ratio of the total energy of all sub-dominant tracks to the total deposited energy of the event (TrackEnergyRatio=1-MTE/Energy), and the blob ratio of the MT (QR\(_i\)). In addition, we also introduce its blob ratio of the second most energetic track (QR\(_2\)).

The last parameter \(\Delta\) aims to identify the de-excitation \(\gamma\) rays even if the energy deposition happens in more than one track. The definition of \(\Delta\) follows EXO-200 [21],

\[
\Delta_i = \min(\{E_j - \gamma_i\}).
\]

In the equation, \(i\) represents the two cases where \(\gamma_1 (\gamma_2) = 760.5 (818.5)\) keV. \(E_j\) iterates all possible combinations of track’s energy of an event.

Figure 4 illustrates the distributions of parameters in MTE ROI [725.66, 788.96] keV. Length cuts \(L^{XZ} \neq 0\) and \(L^{YZ} \neq 0\) are applied to remove very short \(\alpha\) particle tracks originating from the Micromegas’ surface for all the plots in the figure. For projection plane specific parameters, only the ones for the XZ plane is shown. In this MTE ROI, the signal event may include additional electrons and/or \(\gamma\) tracks besides the the 760.5 keV \(\gamma\). Background mostly consists of single \(\gamma\)s. The distinction is demonstrated in the Energy and nTracks distributions. For the same reason, the \(K\) value of signals is close to zero because of the dispersion of signals. The more centered distribution of signal’s \(\Delta\) value in the top right panel is attributed to its particular \(\gamma\)’s energy. Meanwhile, the distributions of the MT length are comparable for signal and background since the events are selected based on MTE. TrackEnergyRatio of background has a prominent peak at zero because most of the background events have only one track at XZ (YZ) plane. Meanwhile, the distribution of TrackEnergyRatio of signals is dominated by the energy of two electrons over Energy. In the case of only one track in background events, QR\(_2\) is not defined and assigned to be -1. On the other hand, a large fraction of background events have QR\(_2\) equalling to 1 because the secondary tracks can be very short and the blobs at the ends cover the whole track. QR\(_2\) of signals peak close to one since the secondary tracks are from two electrons of DBD.
energy spectra of signal and background in logarithmic scale. The signal spectra are shown in linear scale and the background is shown in blue solid line and while these after topological cuts are shown in red solid line. Note that signal spectra are shown in linear scale and the background in logarithmic scale.

Table 2. Significances of MTE, topology, and total cuts in the two MTE ROIs as well as the combined ROI. The last two rows list the total cut efficiencies of signal and background.

| MTE ROI [keV] | [725.7, 789.0] | [789.0, 854.6] | [725.7, 854.6] |
|---------------|----------------|----------------|-----------------|
| MTE           | 3.3            | 2.3            | 3.9             |
| Significance  | 1.7            | 1.9            | 1.8             |
| Efficiency    | 1.2%           | 0.7%           | 1.9%            |
|               | 4.4×10^{-6}    | 2.7×10^{-6}    | 7.1×10^{-6}     |

Table 3. Counts in different MTE ROIs from each background source assuming three years exposure in PandaX-III. The last row lists the projected sensitivities at 90% confidence level.

| MTE ROI [keV] | [725.7, 789.0] | [789.0, 854.6] | [725.7, 854.6] |
|---------------|----------------|----------------|-----------------|
| Liner 238U    | 36             | 22             | 59              |
| Liner 232Th   | 8              | 4              | 12              |
| Liner 226Th   | 260            | 166            | 426             |
| Liner 40K     | 152            | 90             | 242             |
| MM 238U       | 115            | 75             | 190             |
| MM 232Th      | 30             | 15             | 44              |
| SS 238U       | 20             | 12             | 32              |
| SS 232Th      | 17             | 12             | 29              |
| Acrylic 238U  | 378            | 228            | 606             |
| Acrylic 232Th | 94             | 45             | 139             |
| Total Bck     | 1109           | 669            | 1778            |
| Sensitivity [yr] | 3.3×10^{-23} | 2.5×10^{-23} | 4.1×10^{-23}  |

4 Neutrinoless double beta decay to $0^+_1$ excited state

Depending on whether de-excitation $\gamma$ rays deposit their full energy in the active volume of the TPC, we have identified four possible ROIs to search for NLDBD-ES. In all the cases, energy of two electrons is fully contained and recorded. The four ROIs are 878±37.4 keV, 1639.3±51.1 keV, 1697.3±52.0 keV, and 2458.8±62.6 keV, which correspond to events with neither $\gamma$, one 760.5 keV $\gamma$, one 818.5 keV $\gamma$, and both $\gamma$ rays captured. The range of the ROIs are defined as ±2$\sigma$ around the center value, where $\sigma$ is the energy resolution, scaled from an expected...
energy resolution of $\sigma = 1.3\%$ at $Q_{NLDBD} = 2457.8$ keV for PandaX-III. We will use the center value to denote each ROI later in the text.

We define five parameters which are specific to the topological signatures of NLDBD-ES, including the track dispersion (K) parameter calculated with all possible tracks of an event and 4 parameters specific to the main track. The MT-related parameters are MTE, L, TrackEnergyRatio, and Q, which is the smaller of the two end blob energy along MT. In the 878.8 keV ROI, we use all parameters except TrackEnergyRatio. For the other three ROIs, we only use MT-related parameters as input variable for TMVA. Since the energy of two electrons is larger than the other two $\gamma$s in NLDBD-ES, the MT in signal events is the track of two electrons in all four ROIs.

Figure 6 and Figure 7 show the distributions of each input topological parameters used in the 878.8 keV and 1639.3 keV ROIs respectively. For all parameters except TrackEnergyRatio, the distributions of values in X-Z plane are used. The distribution of Q for signals in both figures are similar since those are for the two-electron tracks. For the same reason, the distributions of other 2 MT parameters, L and MTE of signal are almost the same in both ROIs. The small peak near 800 keV in the MTE distributions in Figure 7 is due to wrongly connected electron and $\gamma$ ray tracks.

| ROI [keV]       | 878.8 | 1639.3 | 1697.3 | 2457.8 |
|-----------------|-------|--------|--------|--------|
| Significance    | Topology | 3.0    | 32.6   | 28.7   | 46.5   |
| Efficiency      | Signal  | 39.0%  | 21.2%  | 21.1%  | 47.7%  |
|                 | Background | 1.7×10^{-2}  | 4.3×10^{-2}  | 5.4×10^{-2}  | 1.1×10^{-4}  |

Table 4. Topological significances and related reduction efficiencies (last two rows) of signal and background in each ROI.

In the 878.8 keV ROI, compared to the background events, NLDBD-ES events have larger Q, more concentrated MTE and non-zero K. All the characteristics are due to the fact that signals are two-electron tracks. In the 1639.3 keV ROI, most of the background events have a main track with higher energy and thus longer L, larger MTE, and smaller or even zero TrackEnergyRatio. The distribution of TrackEnergyRatio of signals in the last panel is centered around 0.46, which is expected from the definition.

Table 4 lists the efficiencies and significances of topological cuts in 4 different ROIs and Figure 8 shows the
NLDBD-ES and background spectra before and after topological cuts. With topological cuts, the background has been reduced by 2 to 5 orders of magnitude while keeping NLDBD-ES efficiencies of 21% to 48% in different ROIs. With additional γ rays, the significances of latter three ROIs are better than the first one, as well as those in the DBD-ES cases.

The background counts after energy and topological cuts of 3 years’ exposure in PandaX-III are given in Table 5. The cuts are so effective that we reject almost all the background events in the latter three ROIs.

5 Conclusion and discussion

We have presented the improvement in search sensitivity for (NL)DBD-ES with gaseous detector’s unique capability to record topological information of event trajectories.
jectories. Our study is based on detailed simulation of the PandaX-III detector, with its expected detector performance and background budget. With MTE energy cut and topological characteristics, we may retain 1.9% of the total number of DBD-ES signals while reduce the background by about 6 orders of magnitudes. The estimated sensitivity for DBD-ES with three years’ PandaX-III data reaches 4.1 × 10^{23} yr (90% CL), which represents a factor of 1.8 improvement if we compare that without topological analysis. The sensitivity of the 136Xe NLDBD-ES is 1.7 × 10^{25} yr (90% CL) with 3 years exposure, corresponding to a signal efficiency of 21.3% and background efficiency of 4.3 × 10^{-5} in the 1639.3 keV ROI. Topological analysis improves the search sensitivity of NLDBD-ES by 4.8 times.

Further improvement can be expected in several aspects. For DBD-ES, the search sensitivity of PandaX-III is limited by background. Current theoretical estimations of the half-life of DBD-ES ranges from 10^{23} to 10^{25} yr [27, 28]. Further refinement of the TMVA algorithm parameters and new deep learning techniques may improve the background suppression efficiency and thus the search sensitivity to cover more theoretical range. For NLDBD-ES, the search sensitivity is limited by the number of signals. The current best limit on the 136Xe NLDBD to 0^+ 136Ba half-life is 2.4 × 10^{25} yr (90% CL), given by KamLAND-Zen [29]. A larger gaseous detector would be necessary to further improve the search sensitivity beyond the current limit.

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