Search for two-neutrino double electron capture of \(^{124}\)Xe with XENON100
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Two-neutrino double electron capture is a rare nuclear decay where two electrons are simultaneously captured from the atomic shell. For $^{124}$Xe this process has not yet been observed and its detection would provide a new reference for nuclear matrix element calculations. We have conducted a search for two-neutrino double electron capture from the K-shell of $^{124}$Xe with XENON100.

I. INTRODUCTION

Double electron capture is a rare nuclear decay where a nucleus captures two electrons from the atomic shell

\[ (A, Z) + 2e^- \rightarrow (A, Z - 2) + (2\nu_e). \]  

The two-neutrino mode ($2\nu$2EC) is allowed in the Standard Model while the existence of the lepton number-violating neutrinoless double electron capture ($0\nu$2EC)
would prove the Majorana nature of the neutrino. In 0ν2EC, there is the possibility of a resonant enhancement of the decay rate for decays to excited atomic or nuclear states [1–4]. Due to low isotopic abundances and longer half-lives [5, 6], experimental searches for 0ν2EC are generally not competitive with those for neutrinoless double beta decay (0ν2β) to constrain the effective neutrino mass \(m_{\beta}\beta\) and the neutrino mass hierarchy [7]. The largest uncertainty in the conversion of the half-life of 0ν2β or 0ν2EC to \(m_{\beta}\beta\) is introduced by the calculation of nuclear matrix elements. Although the matrix elements for the two-neutrino and neutrinoless modes of the double electron capture differ, they are based on the same nuclear structure models. A measurement of the 2ν2EC half-life would help to test the accuracy of these models.

So far, 2ν2EC has only been observed for \(^{130}\)Ba in geochemical experiments [8, 9]. In addition, there is an indication for 2ν2EC of \(^{78}\)Kr from a low-background proportional counter [10]. In natural xenon the isotopes \(^{124}\)Xe (\(Q = 2864\) keV [11], abundance 0.095% [12]) and \(^{126}\)Xe (\(Q = 919\) keV [11], abundance 0.089% [12]) can decay via 2ν2EC. However, any signal will be dominated by 124Xe due to the \(Q^2\) dependence of the phase space [13]. In the case of 124Xe, the theoretically calculated branching ratio that the two electrons are captured from the K-shell (2ν2K) is 76.7% [14]. Filling the vacancies of the daughter atom 124Te leads to the emission of X-rays and Auger electrons with a total energy of approximately 64 keV. There is a wide spread in the predicted half-lives of 2ν2EC for 124Xe, from \(\sim 10^{20}\) yr to \(10^{24}\) yr due to different nuclear matrix element calculations [15–20]. Previous searches for 2ν2K of 124Xe have been carried out using a low-background proportional counter with enriched xenon [14, 21] and large-scale liquid xenon detectors [22, 23]. The current best experimental limit on the half-life, \(T_{1/2} > 4.7 \times 10^{21}\) yr (90% confidence level), is set by the XMASS experiment [23].

A limit of \(T_{1/2} > 1.66 \times 10^{21}\) yr (90% confidence level) was derived from previously published XENON100 data [22]. However, the available data was not well suited for a signal search due to the coarse binning. The limit was calculated from the average background rate for the energy region below \(\sim 10\) keV [24], outside the expected 2ν2K signal region and the assumed isotopic abundance of 124Xe did not match the real situation. Here, we improve this study by using the 224.6 live days of XENON100 data and additional insight into the experimental details.

II. THE XENON100 EXPERIMENT

Located at the Laboratori Nazionali del Gran Sasso (LNGS), the XENON100 experiment [25] utilizes a dual-phase xenon time-projection chamber (TPC) in order to search for dark matter particles in form of Weakly Interacting Massive Particles (WIMPs). The TPC contains a total 62 kg of liquid xenon (LXe) in a cylindrical (30.5 cm height and diameter) volume equipped with 178 radio pure photomultiplier tubes (PMTs) placed in the gaseous phase on top and immersed in the LXe at the bottom. The TPC is fully surrounded by an active LXe veto viewed by 64 additional PMTs. If a particle deposits its energy in the LXe, it creates excited atoms and ions leading to the formation of excimers. The de-excitation of these excimers causes prompt scintillation light (S1). A fraction of the electrons generated by the ionization process are drifted towards the gas phase by an applied electric field of 530 V/cm. At the liquid-gas interface they are extracted and accelerated by a strong field of 12 kV/cm. This induces a secondary scintillation signal (S2) which is proportional to the number of generated electrons. Three-dimensional event vertex reconstruction is achieved by obtaining the interaction depth from the time difference of the two signals and by deriving the \((x, y)\)-position from the hit pattern of the S2 signal on the top PMT array. A background-optimized fiducial volume can thus be selected, with a strongly reduced background from external \(\gamma\)-radiation. A detailed description of the detector can be found in Ref. [25].

III. DATA ANALYSIS

Data for the 2ν2K-search consists of 224.6 live days collected between February 28, 2011 and March 31, 2012 using a fiducial target mass of 34 kg. This data set has also been analyzed for different purposes in Refs. [24, 26–29]. The detector was filled with a mixture of natural xenon and xenon depleted in \(^{136}\)Xe and \(^{124}\)Xe, leading to a \(^{124}\)Xe abundance of \(\eta = (8.40 \pm 0.07) \times 10^{-4}\). This corresponds to an absolute amount of about 29 g of \(^{124}\)Xe in the fiducial volume.

The energy calibration uses the S1 and S2 signals from an Americium-Beryllium (\(^{241}\)AmBe) calibration measurement. We employ \(\gamma\)-lines from neutron-activated xenon isotopes at 40 keV and 320 keV (\(^{129}\)Xe), 80 keV (\(^{133}\)Xe), 164 keV (\(^{131m}\)Xe) and 236 keV (\(^{129m}\)Xe). The energy \(E\) was obtained by a linear combination of the S1 and S2 signals measured in photoelectrons (PE), exploiting their anti-correlation [30, 31]

\[
E = W \cdot \left( \frac{S1}{g1} + \frac{S2}{g2} \right)
\]

(2)

\(W\) is the mean energy required to produce a photon or electron and \(g1\) and \(g2\) are detector-specific gain factors. When fixing \(W\) to 13.7 eV [31], the best-fit values of the gain factors are \(g1 = (5.07 \pm 0.03) \times 10^{-2}\) PE/photon and \(g2 = (10.13 \pm 0.07)\) PE/electron. Although the S1 and S2 signals depend on particle type and vary non-linearly with energy, the combined signal provides a common, linear energy scale for both X-rays and Auger electrons at the relevant energies. The energy resolution \(\sigma\) was derived from the same \(\gamma\)-lines and is given by

\[
\sigma(E) = a \cdot \sqrt{E} + b \cdot E
\]

(3)
FIG. 1. Spectrum of remaining events after all cuts. The peak at 164 keV originates from $^{131m}$Xe. The red shaded area indicates the $\pm 3\sigma$ region around the expected 2ν2K peak of $^{124}$Xe.

with $a = (0.405 \pm 0.010) \sqrt{\text{keV}}$ and $b = 0.0261 \pm 0.0008$.

Selection cuts were applied in order to ensure data quality and consistency. Every valid event was required to have exactly one S1 and one corresponding S2. In order to avoid dark count contributions, the S1 had to have a coincident signal in the veto were not considered as this indicates multiple scattering induced by external radiation. The acceptance of each selection cut was calculated analogous to Ref. [32] by determining the fraction of events that passed all selection cuts but the one of interest. The total acceptance $\epsilon$ in the $\pm 3\sigma$-region around the expected signal was found to be $\epsilon = (98.3 \pm 0.1)\%$.

Fig. 1 shows the spectrum after applying all cuts. The peak at 164 keV originates from the de-excitation of the long-lived $^{131m}$Xe ($\tau = 11.8\, \text{d}$) from the neutron calibration before the run. Apart from this peak, the background is nearly constant with an average rate of $5.9 \times 10^{-3}\, \text{events/(keV} \cdot \text{kg} \cdot \text{day})$. This is expected for a background that is dominated by low-energy Compton scatters [33].

To determine the expected mean energy and width of the signal, we calculated the energies and emission probabilities of all X-rays and Auger electrons for a single K-shell vacancy in Te using the RELAX code [34]. The calculation accounts for bound-bound X-rays and electrons which are emitted from transitions within the atomic shell. In addition, it is assumed that the final atom returns to neutrality by filling all remaining vacancies with electrons from the continuum which leads to the emission of free-bound X-rays. The results are summarized in Table I.

The individual quanta emitted in the de-excitation process cannot be resolved due to the limited spatial and timing resolution of the detector. Therefore, the expected signal is a single peak at the sum energy. The RELAX code assumes that the shell binding energies are independent of the ionization of the atom. Therefore, the total emitted energy equals the binding energy of the K-shell of the neutral atom $E_K = 31.8\, \text{keV}$ [35]. In 2ν2K the total emitted energy is given by the double-electron hole energy ($64.457 \pm 0.012)\, \text{keV}$ [36] which is very close to two times the K-shell binding energy $2E_K = 63.6\, \text{keV}$. However, the energies of a small fraction of the emitted quanta are below the xenon excitation threshold of 13.7 eV. According to RELAX, and under the assumption that the quanta emitted in 2ν2K are similar to those generated by two single K-shell vacancies, this leads to an average energy loss of 0.13 keV. Therefore, the 2ν2K peak is expected to be centered at 64.33 keV. To estimate the energy resolution of the signal peak, we take the average energy and number of X-rays and electrons emitted per vacancy as shown in Table I but neglect the contribution from free-bound X-rays. Again, assuming the same de-excitation spectrum as for two single K-captures, we arrive at an energy resolution $\sigma_{\text{sig}}$ of

\[
\sigma_{\text{sig}} = \sqrt{2 \cdot (n_1 \cdot \sigma_{\text{sig}}^2 + n_2 \cdot \sigma_{\text{sig}}^2)},
\]

where $n_1 = 0.96$ and $n_2 = 11.7$ are the average number of X-rays and Auger electrons and $\sigma_{\text{sig}}$ correspond to their respective energy resolution from Eq. (3). This leads to $\sigma_{\text{sig}} = (4.10 \pm 0.27)\, \text{keV}$ compared to $\sigma_{\text{sig}} = (4.93 \pm 0.27)\, \text{keV}$ for a single energy de-position.

The statistical analysis for the signal search uses the Bayesian Analysis Toolkit [37]. The spectrum with a 1 keV binning was fit in the energy range 10–135 keV with a “signal+background” model $f_{\text{sig}}(E)$ and a “background-only” model $f_{\text{bkg}}(E)$

\[
f_{\text{sig}}(E) = \frac{\Gamma \epsilon \text{m} N_A}{\sqrt{2\pi} \sigma_{\text{sig}} M_{\text{Xe}}} \exp \left( -\frac{(E - \mu_{\text{sig}})^2}{2 \sigma_{\text{sig}}^2} \right) + f_{\text{bkg}}(E),
\]

\[
f_{\text{bkg}}(E) = a_{\text{bkg}} E + b_{\text{bkg}},
\]

$E$ is the energy, $\Gamma$ the decay rate, $\epsilon$ the signal acceptance, $n$ the abundance of $^{124}$Xe, $m$ the exposure, $N_A$ Avagadro’s constant, $M_{\text{Xe}}$ the molar mass of xenon, $\mu_{\text{sig}}$ is the mean energy and $\sigma_{\text{sig}}$ the width of the signal peak.

### Table I: Average energies and average number of emitted quanta per K-shell vacancy in Te, as calculated with the RELAX code [34].

<table>
<thead>
<tr>
<th>Energy per Quantum (eV)</th>
<th>Number of Quanta</th>
</tr>
</thead>
<tbody>
<tr>
<td>bound-bound X-rays</td>
<td>25950</td>
</tr>
<tr>
<td>bound-bound electrons</td>
<td>572</td>
</tr>
<tr>
<td>free-bound X-rays</td>
<td>14</td>
</tr>
</tbody>
</table>
TABLE II. Gaussian priors included in the fit to account for systematic uncertainties. The value and uncertainty denote the mean and standard deviation of the Gaussian prior, respectively.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>acceptance $\epsilon$</td>
<td>$(98.3 \pm 0.1)%$</td>
</tr>
<tr>
<td>abundance $\eta$</td>
<td>$(8.40 \pm 0.07) \times 10^{-4}$</td>
</tr>
<tr>
<td>exposure $mt$</td>
<td>$(7636 \pm 45)\text{kg d}$</td>
</tr>
<tr>
<td>peak position $\mu_{\text{sig}}$</td>
<td>$(64.33 \pm 0.37)\text{keV}$</td>
</tr>
<tr>
<td>peak width $\sigma_{\text{sig}}$</td>
<td>$(4.10 \pm 0.27)\text{keV}$</td>
</tr>
</tbody>
</table>

The parameters $a_{\text{bkg}}$ and $c_{\text{bkg}}$ represent the slope and constant term of the background spectrum, respectively. The binned likelihood of the fit assumes independent Poisson fluctuations of the bin entries and is defined as

$$L = \prod_{i=1}^{N_{\text{bin}}} \frac{\lambda_i^{n_i} e^{-\lambda_i}}{n_i!},$$

where $N_{\text{bin}}$ is the total number of bins. $\lambda_i$ is the expected number of events and $n_i$ the observed number of events in the $i$th bin. Systematic uncertainties were included in the fit by Gaussian priors and are summarized in Table II. The uncertainty on the cut acceptance $\epsilon$ is only statistical. For the natural abundance $\eta$, the uncertainty was calculated from the individual uncertainties on the amounts and abundances of the deployed xenon batches. The uncertainty on the exposure $mt$ accounts for the uncertainty in the determination of the fiducial volume due to the limited spatial resolution. Regarding the peak position $\mu_{\text{sig}}$ and width $\sigma_{\text{sig}}$, we included the uncertainties derived from the fits to the energy calibration and resolution. In addition, we added systematic uncertainties of 0.2% and 3% for the peak position and energy resolution, respectively, which were determined from the RELAX calculation. Uniform priors were chosen for the remaining free parameters of the fit, $\Gamma$, $a_{\text{bkg}}$ and $c_{\text{bkg}}$. All fit parameters were constrained to physically allowed positive values. The significance of a possible signal was evaluated by calculating the Bayes Factor [38]

$$BF = \frac{P(f_{\text{bkg}} | \bar{D})}{P(f_{\text{sig}} | \bar{D})},$$

where $P(f | \bar{D})$ is the posterior probability of the model $f$ and $\bar{D}$ is the data.

### IV. RESULTS

The best fits to the spectrum with $f_{\text{sig}}$ and $f_{\text{bkg}}$ are shown in Fig. 2 and the obtained values can be found in Tab. III. The p-values of the “signal+background” and “background-only” fit, calculated as described in Ref. [39], are 0.92 and 0.89, respectively. These values show that the data is well described by both fit models. Since the Bayes Factor is

$$BF = 1.2,$$

and thus favors the “background-only” model, we calculate a lower limit on the half-life. The 90% credibility limit $\Gamma_{\text{lim}}$ on the decay rate is defined as the 90% quantile of the marginalized posterior probability distribution shown in Fig. 3. This leads to a 90% credibility limit on the half-life $T_{1/2}$ of

$$T_{1/2} > \frac{\ln(2)}{\Gamma_{\text{lim}}} = 6.5 \times 10^{20} \text{yr}. $$

The influence of the nuisance parameters on the limit was evaluated by fixing all parameters shown in Table II to their mean values, which weakens the limit by 0.5%. While the binning has only a moderate influence ($\sim 15\%$), decreasing the fit range can worsen the half-life limit by up to a factor of $\sim 2$. The latter comes from the anti-correlation of the parameters $\Gamma$ and $c_{\text{bkg}}$ in Eq. (5). We have checked our result with the Feldman-Cousins procedure [40] using the approach of a simple counting experiment with known background. The number of observed events was derived from the $\pm 3\sigma$ region of the expected $2\nu 2K$ peak, while the number of background events was calculated from the regions left and right of the peak. This gives a lower half-life limit of $7.3 \times 10^{20} \text{yr}$ (90% confidence level) which confirms the result of the full Bayesian analysis.

A comparison of the current experimental half-life limits is shown in Table IV. Since our analysis is more accurate it supersedes the previous limit given in Ref. [22] which made use of the publicly available XENON100 data. The larger mass of the XMASS experiment (835 kg) results in better self-shielding capabilities and consequently a lower background, and thus makes the experiment more sensitive to $2\nu 2K$.

The successor of XENON100, the XENON1T experiment [41], is based on the same detector technology but
with an increased total target mass of 2 t and a reduced background. It is currently in the commissioning phase. The sensitivity of XENON1T for 2ν2K of 124Xe was investigated using the expected background spectrum in a 1 t fiducial volume [41]. We assumed the same energy resolution as in XENON100. This assumption is conservative as the energy resolution is related to the light yield, which is expected to be about a factor of two higher in XENON1T [41]. We used the Bayesian approach for a simple counting experiment with known background to estimate the sensitivity on the half-life in XENON1T.

The likelihood is defined as

\[
L = \frac{(N_{\text{bkg}} + N_{\text{sig}})^{N_{\text{obs}}} e^{-(N_{\text{bkg}} + N_{\text{sig}})}}{N_{\text{obs}}!},
\]

where \(N_{\text{obs}} = N_{\text{bkg}}\) is the expected number of counts in the ±3σ region around the 2ν2K peak, and \(N_{\text{sig}}\) is the number of signal counts. The first is a function of live-time with an expected value of 4.82 counts per day. For the latter a uniform prior was chosen. The limit on the half-life \(T_{1/2}\) was calculated as

\[
T_{1/2} > \frac{\ln(2) n_{\text{nat}} m_t}{M_{Xe} N_{\lim}},
\]

where \(n_{\text{nat}} = 9.52 \times 10^{-4}\) is the natural abundance of 124Xe and \(N_{\lim}\) is the 90% quantile of the posterior distribution for \(N_{\text{sig}}\). The 90% credibility limit on the half-life as a function of measurement time is shown in Fig. 4 for a 1 t fiducial target. With only five live days of XENON1T, we expect to reach a sensitivity exceeding the current best experimental limit. With an exposure of 2 t·yr we expect to reach a half-life limit of \(6.1 \times 10^{22}\) yr.

**V. CONCLUSIONS**

We have conducted a search for 2ν2K of 124Xe using 7636 kg·d of XENON100 data. No significant signal was observed leading to a lower 90% credibility limit on the half-life of \(6.5 \times 10^{20}\) yr. This result supersedes the previ-
ous limit of $> 1.66 \times 10^{21}$ yr [22] from an external analysis of published XENON100 data. We have shown that the XENON1T experiment is expected to probe half-lives up to a value of $6.1 \times 10^{22}$ yr after an exposure of 2 t-yr. Since the XENON1T detector was also designed to measure higher energy signals more accurately than XENON100 it offers the possibility to study neutrinoless double electron capture as well as electron capture with positron emission or double positron decay where the main part of the observable energy is above 1 MeV [42]. Moreover, future multi-ton target experiments such as XMASS-II [23], LZ [22], XENONnT [41] and DARWIN [43] will have the sensitivity to investigate the parameter space even further.

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[34] D. Cullen, Program RELAX: A code designed to calculate atomic relaxation spectra of x-rays and electrons, Tech. Rep. UCRL-ID–110438 (Lawrence Livermore National Laboratory, CA (United States)).