CUORE sensitivity to 0 decay

The MIT Faculty has made this article openly available. Please share how this access benefits you. Your story matters.

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>As Published</td>
<td><a href="http://dx.doi.org/10.1140/EPJC/S10052-017-5098-9">http://dx.doi.org/10.1140/EPJC/S10052-017-5098-9</a></td>
</tr>
<tr>
<td>Publisher</td>
<td>Springer Nature</td>
</tr>
<tr>
<td>Version</td>
<td>Final published version</td>
</tr>
<tr>
<td>Accessed</td>
<td>Tue Jan 08 00:53:30 EST 2019</td>
</tr>
<tr>
<td>Citable Link</td>
<td><a href="http://hdl.handle.net/1721.1/116238">http://hdl.handle.net/1721.1/116238</a></td>
</tr>
<tr>
<td>Terms of Use</td>
<td>Creative Commons Attribution 4.0 International License</td>
</tr>
<tr>
<td>Detailed Terms</td>
<td><a href="http://creativecommons.org/licenses/by/4.0/">http://creativecommons.org/licenses/by/4.0/</a></td>
</tr>
</tbody>
</table>
CUORE sensitivity to $0\nu\beta\beta$ decay

C. Alduino$^1$, K. Alfonso$^2$, D. R. Artusa$^{1,3}$, F. T. Avignone III$^4$, O. Azzolini$^4$, T. I. Banks$^{5,6}$, G. Bari$^7$, J. W. Beeman$^8$, F. Bellini$^{9,10}$, G. Benato$^5$, A. Bersani$^{11}$, M. Biassoni$^{12,13}$, A. Branca$^{14}$, C. Brofferio$^{12,13}$, C. Bucco$^3$, A. Camacho$^4$, A. Caminata$^{11}$, L. Canonica$^{3,15}$, X. G. Cao$^{16}$, S. Capelli$^{12,13}$, L. Cappelli$^3$, L. Carbone$^1$, L. Cardani$^{10}$, P. Carniti$^{12,13}$, N. Casati$^{9,10}$, L. Cassina$^{12,15}$, D. Chiesa$^{12,13}$, N. Chott$^1$, M. Clemenza$^{12,13}$, S. Copello$^{11,17}$, C. Cosmelli$^{9,10}$, O. Cremonesi$^{13,a}$, R. J. Creswick$^1$, J. S. Cushman$^{18}$, A. D'Addabbo$^3$, I. Dafinei$^{10}$, C. J. Davis$^{18}$, S. Dell’Oro$^{3,19}$, M. M. Deninno$^7$, S. Di Domizio$^{11,17}$, M. L. Di Vacri$^{3,20}$, A. Drobizhev$^{5,6}$, D. Q. Fang$^{16}$, M. Faverzani$^{12,13}$, G. Fernandes$^{11,17}$, E. Ferri$^{13}$, F. Ferroni$^{9,10}$, E. Fiorini$^{12,13}$, M. A. Franceschi$^{21}$, S. J. Freedman$^{5,6,b}$, B. K. Fujikawa$^6$, A. Giachero$^{13}$, L. Gironi$^{12,13}$, A. Giuliani$^{22}$, L. Gladstone$^{15}$, P. Gorla$^3$, C. Gott1$^{12,13}$, T. D. Gutierrez$^{23}$, E. E. Halle$^{8,24}$, K. Han$^{35}$, E. Hansen$^{2,15}$, K. M. Heeger$^{18}$, R. Hennings-Yeomans$^{5,6}$, K. P. Hickerson$^2$, H. Z. Huang$^2$, R. Kade$^{26}$, G. Keppe$^{1}$, Yu. G. Kolomensky$^{5,6}$, A. Leduc$^{15}$, C. Lig$^{21}$, K. E. Lim$^{18}$, Y. G. Ma$^{16}$, M. Maino$^{12,13}$, L. Marini$^{11,17}$, M. Martinez$^{9,10,27}$, R. H. Maruyama$^{18}$, Y. Me$^{11}$, N. Moggi$^{7,28}$, S. Morganti$^{10}$, P. J. Mosteiro$^{10}$, T. Napolitano$^{21}$, M. Nastasi$^{12,13}$, C. Nones$^{29}$, E. B. Norman$^{30,31}$, V. Novati$^{22}$, A. Nucciotti$^{12,13}$, T. O’Donnell$^{32}$, J. L. Ouellet$^{15}$, C. E. Pagliarone$^{3,33}$, M. Pallavicini$^{11,17}$, V. Palmieri$^4$, L. Pattavina$^3$, M. Pavan$^{12,13}$, G. Pessina$^{13}$, V. Pettinacci$^{10}$, G. Pipero$^{9,10,c}$, C. Pira$^6$, S. Pirro$^3$, S. Pozzi$^{12,13}$, E. Previtali$^3$, C. Rosenfeld$^1$, C. Rusconi$^{13,1}$, M. Sakai$^2$, S. Sangiorgio$^{30,31}$, D. Santone$^{3,20}$, B. Schmidt$^6$, J. Schmidt$^2$, N. D. Scielzo$^{30}$, V. Singh$^5$, M. Sisti$^{12,13}$, A. R. Smith$^6$, L. Taffarello$^{14}$, M. Tenconi$^{22}$, F. Terranova$^{12,13}$, C. Tomei$^{10}$, S. Trentalange$^2$, M. Vagnani$^{10}$, S. L. Wagaarachchi$^5$, B. S. Wang$^{30,31}$, H. W. Wang$^{16}$, B. Welliver$^6$, J. Wilson$^1$, L. A. Winslow$^{15}$, T. Wise$^{18,34}$, A. Woodcraft$^{35}$, L. Zanotti$^{12,13}$, S. Zimmermann$^{36}$, S. Zucchelli$^{7,37}$

1 Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208, USA
2 Department of Physics and Astronomy, University of California, Los Angeles, CA 90095, USA
3 INFN-Laboratori Nazionali del Gran Sasso, 67010 L’Aquila, Assergi, Italy
4 INFN-Laboratori Nazionali di Legnaro, 35020 Padua, Legnaro, Italy
5 Department of Physics, University of California, Berkeley, CA 94720, USA
6 Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
7 INFN-Sezione di Bologna, Bologna 40127, Italy
8 Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
9 Dipartimento di Fisica, Sapienza Università di Roma, Roma 00185, Italy
10 INFN-Sezione di Roma, Roma 00185, Italy
11 INFN-Sezione di Genova, Genova 16146, Italy
12 Dipartimento di Fisica, Università di Milano-Bicocca, Milano 20126, Italy
13 INFN-Sezione di Milano Bicocca, Milano 20126, Italy
14 INFN-Sezione di Padova, Padova 35131, Italy
15 Massachusetts Institute of Technology, Cambridge, MA 02139, USA
16 Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China
17 Dipartimento di Fisica, Università di Genova, Genova 16146, Italy
18 Department of Physics, Yale University, New Haven, CT 06520, USA
19 INFN-Gran Sasso Science Institute, L’Aquila 67100, Italy
20 Dipartimento di Scienze Fisiche e Chimiche, Università dell’Aquila, L’Aquila 67100, Italy
21 INFN-Laboratori Nazionali di Frascati, Frascati, Rome 00044, Italy
22 Center for Neutrino Physics, CEAC/Saclay, 91191 Gif-sur-Yvette, France
23 Physics Department, California Polytechnic State University, San Luis Obispo, CA 93407, USA
24 Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA
25 Department of Physics and Astronomy, University of California, Berkeley, CA 94720, USA
26 Lawrence Livermore National Laboratory, Livermore, CA 94550, USA
27 Department of Nuclear Engineering, University of California, Berkeley, CA 94720, USA
28 Dipartimento di Scienza per la Qualità della Vita, Alma Mater Studiorum-Università di Bologna, Bologna 47921, Italy
29 Dipartimento di Fisica, Università di Genova, Genova 16146, Italy
30 Department of Nuclear Physics, Texas A&M University, College Station, TX 77843, USA
31 Center for Neutrino Physics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA
Abstract We report a study of the CUORE sensitivity to neutrinoless double beta (0νββ) decay. We used a Bayesian analysis based on a toy Monte Carlo (MC) approach to extract the exclusion sensitivity to the 0νββ decay half-life ($T^{0\nu}_{1/2}$) at 90% credibility interval (CI) – i.e. the interval containing the true value of $T^{0\nu}_{1/2}$ with 90% probability – and the 3σ discovery sensitivity. We consider various background levels and energy resolutions, and describe the influence of the data division in subsets with different background levels. If the background level and the energy resolution meet the expected sensitivity, CUORE will reach a 90% CI exclusion sensitivity of $2\cdot10^{25}$ year with 3 months, and $9\cdot10^{25}$ year with 5 years of live time. Under the same conditions, the discovery sensitivity after 3 months and 5 years will be $7\cdot10^{24}$ year and $4\cdot10^{25}$ year, respectively.

1 Introduction

Neutrinoless double beta decay is a non Standard Model process that violates the total lepton number conservation and implies a Majorana neutrino mass component [1,2]. This decay is currently being investigated with a variety of double beta decaying isotopes. A recent review can be found in Ref. [3]. The cryogenic underground observatory for rare events (CUORE) [4–6] is an experiment searching for 0νββ decay in 130Te. It is located at the Laboratori Nazionali del Gran Sasso of INFN, Italy. In CUORE, 988 TeO$_2$ crystals with natural 130Te isotopic abundance and a 750 g average mass are operated simultaneously as source and bolometric detector for the decay. In this way, the 0νββ decay signature is a peak at the Q-value of the reaction ($Q_{\beta\beta}$, 2527.518 keV for 130Te [7–9]). Bolometric crystals are characterized by an excellent energy resolution (~0.2% Full Width at Half Maximum, FWHM) and a very low background at $Q_{\beta\beta}$, which is expected to be at the $10^{-2}$ cts/(keV-kg-yr) level in CUORE [10].

The current best limit on 0νββ decay in 130Te comes from a combined analysis of the CUORE-0 [11,12] and Cuoricino data [13,14]. With a total exposure of 29.6 kg-year, a limit of $T^{0\nu}_{1/2} > 4.0\cdot10^{24}$ year (90% CI) is obtained [15] for the 0νββ decay half life, $T^{0\nu}_{1/2}$.

After the installation of the detector, successfully completed in the summer 2016, CUORE started the commissioning phase at the beginning of 2017. The knowledge of the discovery and exclusion sensitivity to 0νββ decay as a function of the measurement live time can be exploited to set the criteria for the unblinding of the data and the release of the 0νββ decay analysis results.

In this work, we dedicate our attention to those factors which could strongly affect the sensitivity, such as the background index ($BI$) and the energy resolution at $Q_{\beta\beta}$. In CUORE, the crystals in the outer part of the array are expected to show a higher $BI$ than those in the middle [10]. Considering this and following the strategy already implemented by the GERDA Collaboration [16,17], we show how the division of the data into subsets with different $BI$ could improve the sensitivity.

The reported results are obtained by means of a Bayesian analysis performed with the Bayesian analysis toolkit (BAT) [18]. The analysis is based on a toy-MC approach. At a cost of a much longer computation time with respect to the use of the median sensitivity formula [19], this provides the full sensitivity probability distribution and not only its median value.

In Sect. 2, we review the statistical methods for the parameter estimation, as well as for the extraction of the exclusion and discovery sensitivity. Section 3 describes the experimental parameters used for the analysis while its technical implementation is summarized in Sect. 4. Finally, we present the results in Sect. 5.

2 Statistical method

The computation of exclusion and discovery sensitivities presented here follows a Bayesian approach: we exploit the Bayes theorem both for parameter estimation and model comparison. In this work, we use the following notation:

- $H$ indicates both a hypothesis and the corresponding model;
- $H_0$ is the background-only hypothesis, according to which the known physics processes are enough to explain
the experimental data. In the present case, we expect the 
CUORE background to be flat in a 100 keV region around 
$Q_{\beta\beta}$, except for the presence of a $^{60}$Co summation peak at 
2505.7 keV. Therefore, $H_0$ is implemented as a flat back-
ground distribution plus a Gaussian describing the $^{60}$Co 
peak. In CUORE-0, this peak was found to be centered 
at an energy $1.9 \pm 0.7$ keV higher than that tabulated in 
literature [15]. This effect, present also in Cuoricino [14], 
is a feature of all gamma summation peaks. Hence, we 
will consider the $^{60}$Co peak to be at 2507.6 keV.

- $H_1$ is the background-plus-signal hypothesis, for which 
some new physics is required to explain the data. In our 
case, the physics involved in $H_1$ contains the background 
processes as well as $0\nu\beta\beta$ decay. The latter is modeled 
as a Gaussian peak at $Q_{\beta\beta}$.

- $E$ represents the data. It is a list of $N$ energy bins 
centered at the energy $E_i$ and containing $n_i$ event counts. 
The energy range is [2470; 2570] keV. This is the same range 
used for the CUORE-0 $0\nu\beta\beta$ decay analysis [15], and is 
bounded by the possible presence of peaks from $^{214}$Bi at 
2447.7 keV and $^{208}$Tl X-ray escape at $\sim 2585$ keV [15]. 
While an unbinned fit allows to fully exploit the informa-
tion contained in the data, it can result in a long com-
tputation time for large data samples. Given an energy res-
olution of $\sim 5$ keV FWHM and using a 1 keV bin width, 
the $\pm 3$ sigma range of a Gaussian peak is contained in 
12.7 bins. With the 1 keV binning choice, the loss of infor-
mation with respect to the unbinned fit is negligible.

- $\Gamma^{0\nu}$ is the parameter describing the $0\nu\beta\beta$ decay rate for 
$H_1$:

$$\Gamma^{0\nu} = \ln \frac{2}{\Gamma^{1/2}} \quad (1)$$

- $\theta$ is the list of nuisance parameters describing the back-
ground processes in both $H_0$ and $H_1$;
- $\Omega$ is the parameter space for the parameters $\theta$.

2.1 Parameter estimation

We perform the parameter estimation for a model $H$ through 
the Bayes theorem, which yields the probability distribu-
tion for the parameters based on the measured data, under 
the assumption that the model $H$ is correct. In the $0\nu\beta\beta$ 
analysis, we are interested in the measurement of $\Gamma^{0\nu}$ for 
the hypothesis $H_1$. The probability distribution for the parameter 
set ($\Gamma^{0\nu}, \theta$) is:

$$P \left( \Gamma^{0\nu}, \theta \mid E, H_1 \right) = \frac{P \left( E \mid \Gamma^{0\nu}, \theta, H_1 \right) \pi \left( \Gamma^{0\nu} \right) \pi(\theta)}{\int_\Omega \int_0^\infty P \left( E \mid \Gamma^{0\nu}, \theta, H_1 \right) \pi \left( \Gamma^{0\nu} \right) \pi(\theta) \, d\Gamma^{0\nu} \, d\theta}, \quad (2)$$

The numerator contains the conditional probability $P \left( E \mid \Gamma^{0\nu}, \theta, H_1 \right)$ of finding the measured data $E$ given 
the model $H_1$ for a set of parameters ($\Gamma^{0\nu}, \theta$), times the prior probability $\pi$ for each of the considered parameters. The prior 
probability has to be chosen according to the knowledge available 
before the analysis of the current data. For instance, the prior 
for the number of signal counts $\Gamma^{0\nu}$ might be based on the 
half-life limits reported by previous experiments while the 
for the background level in the region of interest (ROI) 
could be set based on the extrapolation of the background 
measured outside the ROI. The denominator represents the 
overall probability to obtain the data $E$ given the hypothesis 
$H_1$ and all possible parameter combinations, $P \left( E \mid H_1 \right)$.

The posterior probability distribution for $\Gamma^{0\nu}$ is obtained 
via marginalization, i.e. integrating $P \left( \Gamma^{0\nu}, \theta \mid E, H_1 \right)$ over 
all nuisance parameters $\theta$:

$$P \left( \Gamma^{0\nu} \mid H_1, E \right) = \int_\Omega P \left( \Gamma^{0\nu}, \theta \mid E, H_1 \right) d\theta \quad (3)$$

For each model $H$, the probability of the data given the 
model and the parameters has to be defined. For a fixed set of 
experimental data, this corresponds to the likelihood func-
tion [20]. Dividing the data into $N_d$ subsets with index $d$ 
characterized by different background levels, and consider-
ing a binned energy spectrum with $N$ bins and a number $n_{di}$ 
of events in the bin $i$ of the $d$ subset spectrum, the likelihood 
function is expressed by the product of a Poisson term for each 
bin $d$:

$$P \left( E \mid \Gamma^{0\nu}, \theta, H \right) = L \left( E \mid \Gamma^{0\nu}, \theta, H \right) = \prod_{d=1}^{N_d} \prod_{i=1}^{N} e^{-\lambda_{di}} \frac{\lambda_{di}^{n_{di}}}{n_{di}!}, \quad (4)$$

where $\lambda_{di}$ is the expectation value for the bin $d, i$. The best-fit 
is defined as the set of parameter values ($\Gamma^{0\nu}, \theta$) for which 
the likelihood is at its global maximum. In the practical case, 
we perform the maximization on the log-likelihood

$$\ln L \left( E \mid \Gamma^{0\nu}, \theta, H \right) = \sum_{d=1}^{N_d} \sum_{i=1}^{N} (-\lambda_{di} + \ln n_{di}^{\lambda_{di}}), \quad (5)$$

where the additive terms $- \ln (n_{di}!)$ are dropped from the 
calculation.

The difference between $H_0$ and $H_1$ is manifested in the 
formulation of $\lambda_{di}$. As mentioned above, we parametrize $H_0$ 
with a flat distribution over the considered energy range, i.e. 
[2470; 2570] keV:

$$f_{bk}(E) = \frac{1}{E_{max} - E_{min}} \quad (6)$$
plus a Gaussian distribution for the $^{60}$Co peak:

$$f_{Co}(E) = \frac{1}{\sqrt{2\pi} \sigma} \exp\left(-\frac{(E - \mu_{Co})^2}{2\sigma^2}\right).$$  (7)

The expected background counts in the bin $d_i$ corresponds to the integral of $f_{bkg}(E)$ in the bin $d_i$ times the total number of background counts $M_d^{bkg}$ for the subset $d$:

$$\lambda_{d_i}^{bkg} = \int_{E_{d_i}^{\min}}^{E_{d_i}^{\max}} E M_d^{bkg} f_{bkg}(E) dE$$  (8)

where $E_{d_i}^{\min}$ and $E_{d_i}^{\max}$ are the left and right margins of the energy bin $d_i$, respectively. Considering bins of size $\delta E_{d_i}$ and expressing $M_d^{bkg}$ as a function of the background index $B|_{d_i}$, of the total mass $m_d$ and of the measurement live time $t_d$, we obtain:

$$\lambda_{d_i}^{bkg} = B|_{d_i} \cdot m_d \cdot t_d \cdot \delta E_{d_i}.\quad (9)$$

Similarly, the expectation value for the $^{60}$Co distribution on the bin $d_i$ is:

$$\lambda_{d_i}^{Co} = \int_{E_{d_i}^{\min}}^{E_{d_i}^{\max}} \frac{M_d^{Co}}{\sqrt{2\pi} \sigma} \exp\left(-\frac{(E - \mu_{Co})^2}{2\sigma^2}\right) dE.$$  (10)

where $M_d^{Co}$ is the total number of $^{60}$Co events for the subset $d$ and can be redefined as function of the $^{60}$Co event rate, $R_d^{Co}$:

$$M_d^{Co} = R_d^{Co} \cdot m_d \cdot t_d.\quad (11)$$

The total expectation value $\lambda_{d_i}$ for $H_0$ is then:

$$\lambda_{d_i} = \lambda_{d_i}^{bkg} + \lambda_{d_i}^{Co}.\quad (12)$$

In the case of $H_1$ an additional expectation value for $0\nu\beta\beta$ decay is required:

$$\lambda_{d_i}^{0\nu} = \int_{E_{d_i}^{\min}}^{E_{d_i}^{\max}} \frac{M_d^{0\nu}}{\sqrt{2\pi} \sigma} \exp\left(-\frac{(E - Q_{\beta\beta})^2}{2\sigma^2}\right) dE.$$  (13)

The number of $0\nu\beta\beta$ decay events in the subset $d$ is:

$$M_d^{0\nu} = \Gamma^{0\nu} \frac{N_A}{m_A} \cdot f_{130} \cdot \varepsilon_{\text{tot}} \cdot m_d \cdot t_d,\quad (14)$$

where $N_A$ is the Avogadro number, $m_A$ and $f_{130}$ are the molar mass and the isotopic abundance of $^{130}$Te and $\varepsilon_{\text{tot}}$ is the total efficiency, i.e. the product of the containment efficiency $\varepsilon_{MC}$ (obtained with MC simulations) and the instrumental efficiency $\varepsilon_{\text{instr}}$.

### 2.2 Exclusion sensitivity

We compute the exclusion sensitivity by means of the 90% CI limit. This is defined as the value of $T_{1/2}^{0\nu}$ corresponding to the 90% quantile of the posterior $\Gamma^{0\nu}$ distribution:

$$\Gamma_{1/2}^{0\nu} (90\%\ CI) = T_{1/2}^{0\nu} : \int_0^{\ln 2/T_{1/2}^{0\nu}} P(\Gamma^{0\nu} | H_1, E) d\Gamma^{0\nu} = 0.9.\quad (15)$$

An example of posterior probability for $\Gamma^{0\nu}$ and the relative 90% CI limit is shown in Fig. 1. Top. Flat prior distributions are used for all parameters, as described in Sect. 3.

In the Bayesian approach, the limit is a statement regarding the true value of the considered physical quantity. In our case, a 90% CI limit on $T_{1/2}^{0\nu}$ is to be interpreted as the value above which, given the current knowledge, the true value of $T_{1/2}^{0\nu}$ lies with 90% probability. This differs from a frequentist 90% C.L. limit, which is a statement regarding the possible results of the repetition of identical measurements and should be interpreted as the value above which the best-fit value of $T_{1/2}^{0\nu}$.
In order to extract the exclusion sensitivity, we generate a set of $N$ toy-MC spectra according to the background-only model, $H_0$. We then fit spectra with the background-plus-signal model, $H_1$, and obtain the $T_{1/2}^{0\nu}$ (90\% CI) distribution (Fig. 1, bottom). Its median $\hat{T}_{1/2}^{0\nu}$ is referred as the median sensitivity. For a real experiment, the experimental $T_{1/2}^{0\nu}$ limit is expected to be above/below $\hat{T}_{1/2}^{0\nu}$ (90\% CI) with 50\% probability. Alternatively, one can consider the mode of the distribution, which corresponds to the most probable $T_{1/2}^{0\nu}$ limit.

The exact procedure for the computation of the discovery sensitivity is the following:

\begin{itemize}
\item for each subset, we generate a random number of background events $n_{bkg}^{d\nu\nu}$ according to a Poisson distribution with mean $\lambda_d^{bkg}$;
\item for each subset, we generate $N_{d\nu\nu}^{bkg}$ events with an energy randomly distributed according to $f_{bkg}(E)$;
\item we repeat the procedure for the $\nu^{\beta\beta}$ contribution;
\item we fit the toy-MC spectrum with the $H_1$ model (Eq. 2), and marginalize the likelihood with respect to the parameters $B_{1\nu}$ and $R_{d\nu\nu}^{\nu\beta\beta}$ (Eq. 3);
\item we extract the 90\% CI limit on $T_{1/2}^{0\nu}$;
\item we repeat the algorithm for $N$ toy-MC experiments, and build the distribution of $T_{1/2}^{0\nu}$ (90\% CI).
\end{itemize}

### 2.3 Discovery sensitivity

The discovery sensitivity provides information on the required strength of the signal amplitude for claiming that the known processes alone are not sufficient to properly describe the experimental data. It is computed on the basis of the comparison between the background-only and the background-plus-signal models. A method for the calculation of the Bayesian discovery sensitivity was introduced in Ref. [21]. We report it here for completeness.

In our case, we assume that $H_0$ and $H_1$ are a complete set of models, for which:

$$P(H_0|E) + P(H_1|E) = 1.$$ \hfill (16)

The application of the Bayes theorem to the models $H_0$ and $H_1$ yields:

$$P(H_0|E) = \frac{P(E|H_0)\pi(H_0)}{P(E)}$$

$$P(H_1|E) = \frac{P(E|H_1)\pi(H_1)}{P(E)}.$$ \hfill (17)

In this case, the numerator contains the probability of measuring the data $E$ given the model $H$:

$$P(E|H_0) = \int_\Omega P(E|\theta, H_0)\pi(\theta) \, d\theta$$

$$P(E|H_1) = \int_\Omega \int_0^\infty P(E|\Gamma^{0\nu}, \theta, H_1) \times \pi(\Gamma^{0\nu}) \pi(\theta) \, d\theta \, d\Gamma^{0\nu},$$ \hfill (18)

while the prior probabilities for the models $H_0$ and $H_1$ can be chosen as 0.5 so that neither model is favored.

The denominator of Eq. 17 is the sum probability of obtaining the data $E$ given either the model $H_0$ or $H_1$:

$$P(E) = P(E|H_0)\pi(H_0) + P(E|H_1)\pi(H_1).$$ \hfill (19)

At this point we need to define a criterion for claiming the discovery of new physics. Our choice is to quote the 3$\sigma$ (median) discovery sensitivity, i.e. the value of $T_{1/2}^{0\nu}$ for which the posterior probability of the background-only model $H_0$ given the data is smaller than 0.0027 in 50\% of the possible experiments. In other words:

$$\hat{T}_{1/2}^{0\nu}(3\sigma) = T_{1/2}^{0\nu} : P(H_0|E) < 0.0027$$

for $N/2$ experiments. \hfill (20)

The detailed procedure for the determination of the discovery sensitivity is:

\begin{itemize}
\item we produce a toy-MC spectrum according to the $H_1$ model with an arbitrary value of $T_{1/2}^{0\nu}$;
\item we fit the spectrum with both $H_0$ and $H_1$;
\item we compute $P(H_0|E)$;
\item we repeat the procedure for $N$ toy-MC spectra using the same $T_{1/2}^{0\nu}$;
\item we repeat the routine with different values of $T_{1/2}^{0\nu}$ until the condition of Eq. 20 is satisfied. The iteration is implemented using the bisection method until a $5 \cdot 10^{-5}$ precision is obtained on the median $P(H_0|E)$.
\end{itemize}

### 3 Experimental parameters

The fit parameters of the $H_1$ model are $B_{1\nu}$, $R_{d\nu\nu}^{\nu\beta\beta}$ and $\Gamma^{0\nu}$, while only the first two are present for $H_0$. If the data are divided in subsets, different $B_{1\nu}$ and $R_{d\nu\nu}^{\nu\beta\beta}$ fit parameter are considered for each subset. On the contrary, the inverse $0\nu\beta\beta$ half-life is common to all subsets.

Prior to the assembly of the CUORE crystal towers, we performed a screening survey of the employed materials [22–29]. From these measurements, either a non-zero activity was obtained, or a 90\% confidence level (C.L.) upper limit was set. Additionally, the radioactive contamination of the crystals and holders was also obtained from the CUORE-0 back-
the normalization of the simulated spectra. We then computed measurements and of the CUORE-0 background model for the parameters. In particular, the prior distribution for different BI of exposed faces. Correspondingly, they are characterized by crystals can be divided in 4 subsets with different numbers per only on 2 sides. Considering the CUORE geometry, the copper shield, were characterized by a larger background uppermost and lowermost levels, which had 3 sides facing was already observed in CUORE-0, where the crystals in the copper surface are expected to have a larger Q\beta\beta contribution normalized to the 90% C.L. limit of its posterior distribution. This corresponds to the most conservative choice. Any other reasonable prior, e.g. a scale invariant prior on \Gamma^{0v}, would yield a stronger limit. A different prior choice based on the real characteristic of the experimental spectra might be more appropriate for BI and \textit{R}^{Co} in the analysis of the CUORE data. For the time being the lack of data prevents the use of informative priors. As a cross-check, we performed the analysis using the BI and \textit{R}^{Co} rate uncertainties obtained by the background budget as the \sigma of a Gaussian prior. No significant difference was found on the sensitivity band because the Poisson fluctuations of the generated number of background and \textit{R}^{Co} events are dominant for the extraction of the \Gamma^{0v} posterior probability distribution.

Table 3 lists the constant quantities present in the formulation of \textit{H}_0 and \textit{H}_1. All of them are fixed, with the exception of the live time \textit{t} and the FWHM of the 0\nu\beta\beta decay and \textit{R}^{Co} Gaussian peaks. We perform the analysis with a FWHM of 5 and 10 keV, corresponding to a \sigma of 2.12 and 4.25 keV, respectively. Regarding the efficiency, while in the toy-MC production the BI and \textit{R}^{Co} are multiplied by the instrumental efficiency,\footnote{The containment efficiency is already encompassed in BI and \textit{R}^{Co} \cite{10}.} in the fit the total efficiency is used. This is the product of the containment and instrumental efficiency. Also in this case, we use the same value as for CUORE-0, i.e. 81.3% \cite{15}. We evaluate the exclusion and discovery sensitivities for different live times, with \textit{t} ranging from 0.1 to 5 year and using logarithmically increasing values: \textit{t}_i = 1.05 \cdot \textit{t}_{i-1}.

### 4 Fit procedure

We perform the analysis with the software BAT v1.1.0-DEV \cite{21}, which internally uses CUBA \cite{31} v4.2 for the integration of multi-dimensional probabilities and the Metropolis-Hastings algorithm \cite{32} for the fit. The computation time depends on the number of samples drawn from the considered probability distribution.

For the exclusion sensitivity, we draw 10\textsuperscript{5} likelihood samples for every toy-MC experiment, while, due to the higher computational cost, we use only 10\textsuperscript{3} for the discovery sensitivity.

For every combination of live time, BI and energy resolution, we run 10\textsuperscript{5} (10\textsuperscript{3}) toy-MC experiments for the exclusion (discovery) sensitivity study. In the case of the discovery sensitivity, we chose the number of toy-MC experiments as the minimum for which a 2% relative precision was achievable on the median sensitivity. For the exclusion sensitivity, it was possible to increase both the number of toy-MC experiments and iterations, with a systematic uncertainty on the median sensitivity at the per mil level.

### Table 1: Input parameters for the production of toy-MC spectra

\begin{tabular}{lcc}
<table>
<thead>
<tr>
<th>BI [cts/keV-kg-year]</th>
<th>\textit{R}^{Co} [cts/kg-year]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1.02 \pm 0.03\text{stat})^{-0.23}_{+0.19} \text{syst} \times 10^{-2})</td>
<td>0.428</td>
</tr>
</tbody>
</table>
\end{tabular}

A major ingredient of a Bayesian analysis is the choice of the priors. In the present case, we use a flat prior for all parameters. In particular, the prior distribution for \Gamma^{0v} is flat between zero and a value large enough to contain >99.999% of its posterior distribution. This corresponds to the most conservative choice. Any other reasonable prior, e.g. a scale invariant prior on \Gamma^{0v}, would yield a stronger limit.
5 Results and discussion

5.1 Exclusion sensitivity

The distributions of 90% CI limit as a function of live time with no data subdivision are shown in Fig. 2. For all $BI$ values and all live times, the FWHM of 5 keV yields a $\sim$45% higher sensitivity with respect to a 10 keV resolution. The median sensitivity after 3 months and 5 years of data collection in the two considered cases are reported in Table 4. The dependence of the median sensitivity on live time is typical of a background-dominated experiments: namely, CUORE expects about one event every four days in a 692 kg detector (78% after 3 months to 3% after 5 years). One remark has to be done concerning the values reported in [19]: there we gave a 90% C.I. exclusion sensitivity of $9.3 \cdot 10^{-5}$ year with 5 year of live time. This is $\sim$5% higher than the result presented here and is explained by the use of a different total efficiency: 87.4% in [19] and 81.3% in this work.

We then extract the exclusion sensitivity after dividing the crystals in 4 subsets, as described in Sect. 3. The median exclusion sensitivity values after 3 months and 5 years of data collection with one and 4 subsets are reported in Table 4. The division in subsets yields only a small improvement (at the percent level) in median sensitivity. Based on this results only, one would conclude that dividing the data into subsets with different $BI$ is not worth the effort. This conclusion is not always true, and strongly relies on the exposure and $BI$ of the considered subsets. As an example, we repeated a toy analysis assuming a $BI$ of $10^{-2}$ cts/(keV·kg·yr), and with two subsets of equal exposure and $BI$ 0.5 $\cdot$ $10^{-2}$ cts/(keV·kg·yr) and 1.5 $\cdot$ $10^{-2}$ cts/(keV·kg·yr), respectively. In this case, the division of the data in to two subsets yields a $\sim$10% improvement after 5 year of data taking. Hence, the data subdivision is a viable option for the final analysis, whose gain strongly depends on the experimental BI of each channel. Similarly, we expect the CUORE bolometers to have different energy resolutions; in CUORE-0, these ranged from $\sim$3 keV to $\sim$20 keV FWHM [34]. In the real CUORE analysis a further splitting of the data can be done by grouping the channels with similar FWHM, or by keeping every channels separate. At the present stage it is not possible to make reliable predictions for the FWHM distribution among the crystals, so we assumed an average value (of 5 or 10 keV) throughout the whole work.

Ideally, the final CUORE $0\nu\beta\beta$ decay analysis should be performed keeping the spectra collected by each crystal separate, additionally to the usual division of the data into data sets comprised by two calibration runs [15]. Assuming an average frequency of one calibration per month, the total number of energy spectra would be $\sim$6 $\cdot$ 10^4. Assuming a different but stationary $BI$ for each crystal, and using the same $^{60}$Co rate for all crystals, the fit model would have $\sim$10^5 parameters. This represents a major obstacle for any existing implementation of the Metropolis-Hastings or Gibbs sampling algorithm. A possible way to address the problem might be the

---

2 See the discussion of the pulls for a more detailed explanation.
We perform two further cross-checks in order to investigate the relative importance of the flat background and the 60Co peak. In the first scenario we set the $BI$ to zero, and do the same for the 60Co rate in the second one. In both cases, the difference with respect to the standard scenario is below 1%. We can conclude that the 60Co peak with an initial rate of 0.428 cts/(kg yr) is not worrisome for a resolution of up to 10 keV, and that the lower sensitivity obtained with 10 keV FWHM with respect to the 5 keV case is ascribable to the relative amplitude of $\lambda_{\nu}^{bg}$ and $\lambda_{\nu}^{0}$ only (Eqs. 9 and 13). This is also confirmed by the computation of the sensitivity for the optimistic scenario without the 60Co rate to zero. In both cases, the difference with respect to the standard scenario is below 1%.

We test the fit correctness and bias computing the pulls, i.e. the normalized residuals, of the number of counts assigned to each of the fit components. Denoting with $N^{bg}$ and $N^{Co}$ the number of generated background and 60Co events, respectively, and with $M^{bg}$ and $M^{Co}$ the corresponding number of reconstructed events, the pulls are defined as:

$$r_{bg}(Co) = \frac{M^{bg}(Co) - N^{bg}(Co)}{\sigma_{M^{bg}(Co)}},$$

(21)

where $\sigma_{M^{bg}(Co)}$ is the statistical uncertainty on $M^{bg}(Co)$ given by the fit.

For an unbiased fit, the distribution of the pulls is expected to be Gaussian with a unitary root mean square (RMS). In the case of exclusion sensitivity, we obtain $r_{bg} = -0.2 \pm 0.4$ and $r_{Co} = 0.1 \pm 0.5$ for all live times. The fact that the effect on the median sensitivity. The different colored areas depict the ranges containing the 68.3, 95.5 and 99.7% of the toy-MC experiments. They are computed for each live time value separately as described in Fig. 1, bottom. We also show the sensitivity computed as in [19] in dark green. The horizontal green line at 4·10^24 year corresponds to the limit obtained with CUORE-0 and Cuoricino [15].
pull distributions are slightly shifted indicates the presence of a bias. Its origin lies in the Bayesian nature of the fit and is that all fit contributions are constrained to be greater than zero. We perform a cross-check, by extending the range of all parameters ($B_I$, $R^{Co}$ and $\Gamma^{0\nu}$) to negative values. Under this condition, the bias disappears. In addition to this, an explanation is needed for the small RMS of the pull distributions. This is mainly due to two effects: first, the toy-MC spectra are generated using $H_0$, while the fit is performed using $H_1$; second, the statistical uncertainties on all parameters are larger than the Poisson uncertainty on the number of generated events. To confirm the first statement, we repeat the fit using $H_0$ instead of $H_1$ and we obtain pulls with zero mean and an RMS $\sim$0.8, which is closer to the expected value. Finally, we compare the parameter uncertainty obtained from the fit with the Poisson uncertainty for the equivalent number of counts, and we find that the difference is of $O$(20%).

5.2 Discovery sensitivity

The extraction of the discovery sensitivity involves fits with the background-only and the background-plus-signal models. Moreover, two multi-dimensional integrations have to be performed for each toy-MC spectrum, and a loop over the $0
\nu\beta\beta$ decay half-life has to be done until the condition of Eq. 20 is met. Due to the high computation cost, we compute the 3 $\sigma$ discovery sensitivity for a FWHM of 5 and 10 keV with no crystal subdivision. As shown in Fig. 3, with a 5 keV energy resolution CUORE has a 3 $\sigma$ discovery sensitivity superior to the limit obtained from the combined analysis of CUORE-0 and CUORICINO data [15] after less than one month of operation, and reaches $3.7 \cdot 10^{25}$ year with 5 year of live time.

Also in this case, the pulls are characterized by an RMS smaller than expected, but no bias is present due to the use of $H_1$ for both the generation and the fit of the toy-MC spectra.

6 Conclusion and outlook

We implemented a toy-MC method for the computation of the exclusion and discovery sensitivity of CUORE using a Bayesian analysis. We have highlighted the influence of the $B_I$ and energy resolution on the exclusion sensitivity, showing how the achievement of the expected 5 keV FWHM is desirable. Additionally, we have shown how the division of the data into subsets with different $B_I$ could yield an improvement in exclusion sensitivity.

Once the CUORE data collection starts and the experimental parameters are available, the sensitivity study can be repeated in a more detailed way. As an example, non-Gaussian spectral shapes for the $0
\nu\beta\beta$ decay and $^{60}$Co peaks can be used, and the systematics of the energy reconstruction can be included.

Acknowledgements The CUORE Collaboration thanks the directors and staff of the Laboratori Nazionali del Gran Sasso and the technical staff of our laboratories. CUORE is supported by the Istituto Nazionale di Fisica Nucleare (INFN); The National Science Foundation under Grant Nos. NSF-PHY-0605119, NSF-PHY-0500337, NSF-PHY-0855314, NSF-PHY-0902171, NSF-PHY-0969852, NSF-PHY-1307204, NSF-PHY-1314881, NSF-PHY-1401832, and NSF-PHY-1404205; The Alfred P. Sloan Foundation; The University of Wisconsin Foundation; Yale University; The US Department of Energy (DOE) Office of Science under Contract Nos. DE-AC02-05CH1-1231, DE-AC52-07NA27344, and DE-SC0012654; The DOE Office of Science, Office of Nuclear Physics under Contract Nos. DE-FG02-08ER41551 and DE-FG03-08ER41138; The National Energy Research Scientific Computing Center (NERSC).

Open Access This article is distributed under the terms of the Creative Commons Attribution 4.0 International License (http://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution, and reproduction in any medium, provided you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made. Funded by SCOAP3.

References

doi:10.1140/epjc/s10052-017-5080-6
11. C. Alduino et al. [CUORE Collaboration], JINST 11, P07009 (2016)
14. E. Andreotti et al. [Cuoricino Collaboration], Astropart. Phys. 34, 822 (2011)
arXiv:1109.0494v3
20. F. James, Statistical Methods in Experimental Physics, 2nd edn.
(Word Scientific, Singapore, 2006)