

# Internal calibration of the LUX detector using tritiated methane

LUX Collab List

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## Abstract

We have developed a new method to inject tritiated methane into detectors which utilize liquid and gas phase noble gases as an internal calibration source. The ability to use internal calibration sources is critical in large scale particle physics experiments. Our system uses volume sharing techniques to inject a finely tuned amount of tritiated methane into the detector, and uses a zirconium getter to remove the tritiated methane after the calibration has been completed. We present data from the LUX detector to prove our tritiated methane system can calibrate electron recoil events and remove the internal source to undetectable levels afterward.

## I. Introduction

The LUX collaboration recently reported results from its first underground science run, placing new constraints on WIMP dark matter with masses between 6 GeV and 1 TeV[?]. LUX is a large dual-phase liquid xenon (LXe) time projection chamber (TPC) with an active mass of 270 kg. The primary scintillation light from particle interactions (S1) is collected by two arrays of photomultiplier tubes (PMTs) at the top and bottom of the detector, and the charge signal is converted to light via secondary scintillation at the anode (S2). Measurement of both S1 and S2 allows the event to be located in all three dimensions, and allows discrimination between nuclear recoil (NR) events from electron recoil (ER) events via the ratio (S2/S1).

One of the primary advantages of the liquid TPC technology is its high efficiency for the rejection of external gamma backgrounds via self-shielding. This

has enabled the exploration of three orders of magnitude in WIMP-nucleon cross-section over the last decade. On the other hand, self-shielding also reduces the effectiveness of external gamma sources such as  $^{137}\text{Cs}$  or  $^{228}\text{Th}$  for detector calibration purposes, particularly in the center of the detector and at the low energies relevant for dark matter. In the case of LUX, external gamma source are unable to produce a useful rate of ER calibration events in the fiducial region.

To address this issue, internal calibration sources that can be dissolved into the liquid xenon and thereby defeat its self-shielding have been developed[?, ?]. LUX has deployed two such internal calibration sources; the first based upon  $^{83\text{m}}\text{Kr}$ , and the second based upon tritium ( $^3\text{H}$ ).  $^{83\text{m}}\text{Kr}$  is a source of two internal conversion electrons at energies of 9.4 keVee and 32.1 keVee separated in time by an intermediate state with a half life of 154 ns. Because it produces two lines in the energy spectrum,  $^{83\text{m}}\text{Kr}$

is well adapted for tracking the spatial and time dependence of the S1 and S2 signals. However, because both  $^{83m}\text{Kr}$  electrons are above the energy range of interest for dark matter (1.3 - 8 keVee), and because the S2 signals from the two electrons generally overlap with each other in the detector,  $^{83m}\text{Kr}$  is less useful for constraining the electron recoil (ER) band of the S2/S1 discriminant.

In this article we describe the development and use of the LUX tritium source, which plays a complementary role to the  $^{83m}\text{Kr}$  source. Unlike  $^{83m}\text{Kr}$ , tritium is a single-beta emitter, with a Q value of 18.6 keVee. Its spectral maximum is at 2.5 keVee, and 75% of its beta decays are below 8 keVee. This allows the detector's ER band to be precisely characterized in a short calibration run without saturating the DAQ. In addition, the tritium spectrum has a finite decay rate extending down to zero keVee, allowing the threshold response of the detector to be studied.

Unlike  $^{83m}\text{Kr}$ , however, tritium is long-lived, with a half-life of 12.3 years, compared to 1.8 hours for  $^{83m}\text{Kr}$ . So while the  $^{83m}\text{Kr}$  is naturally removed from the detector after roughly a day, the tritium must be removed from the liquid xenon by purification. Secondly, tritium must be introduced into the detector in a manner which will not impair the charge or light collection properties of the detector. This is less of a concern with  $^{83m}\text{Kr}$ , because it can be passed through the LUX getter prior to entering the detector owing to its noble nature.

Tritiated methane ( $\text{CH}_3\text{T}$ ) was chosen as the appropriate host molecule to deliver the activity into LUX. Methane has several desirable chemical and physical properties compared to  $\text{T}_2$ : first, its diffusion constant (D) times solubility (K) is ten times smaller in common LUX materials such as teflon (PTFE) and polyethylene (PE), mitigating the problem of back-diffusion of activity into the liquid xenon after purifi-

cation; it is chemically inert, so it is not expected to adhere to surfaces (as the  $\text{T}_2$  molecule is known to do), and it is consistent with good charge transport in liquid xenon.

Our goal was to develop a ( $\text{CH}_3\text{T}$ ) source which could be safely injected into LUX and removed such that any residual activity that remained (due to back-diffusion from plastics or inefficient purification) should be no more than  $0.33 \mu\text{Bq}$ , which is 5% of the LUX ER background rate design goal for a 30,000 kg-days exposure. We desired to collect a LUX calibration dataset of  $\sim 15,000$  tritium events, roughly a factor of 100 larger than the number of expected ER background events in LUX.

## II. Tritiated Methane Removal

$\text{CH}_3\text{T}$  removal efficiency of zirconium getters had previously been studied at the University of Maryland. It was found that ..... [ATTILA'S PAPER]. Additionally, a table top gaseous xenon system was developed at the University of Maryland to examine the effects of residuals contamination after injecting  $\text{CH}_3\text{T}$ . It was found that a SAES MC1-905F methane purifier placed in series immediately after the  $\text{CH}_3\text{T}$  source bottle was required to prevent tritium from non-methane species from contaminating the plumbing. Using the result of these two studies, a small scale tritiated methane injection system was integrated into a liquid xenon system at the University of Maryland. After cumulatively injecting over 68,000 Bq of observed  $\text{CH}_3\text{T}$  we were able to achieve purification efficiencies ranging from 99.983% - 100%, with an average purification efficiency of 99.999% in our liquid experiments, where we define our purification efficiency to be

$$\text{Purification Efficiency} = 1 - \frac{A-B}{I-B},$$

where  $A$  is the background event rate after injecting  $\text{CH}_3\text{T}$ ,  $B$  is the background event rate prior to injecting  $\text{CH}_3\text{T}$ , and  $I$  is the injected  $\text{CH}_3\text{T}$  activity as observed by out PMTs. The liquid system was also used to study the effect of out gassing from plastics on the residual background rate after a  $\text{CH}_3\text{T}$  injection. We found that the addition of plastic curtains around our PMTs does not impair our ability to remove  $\text{CH}_3\text{T}$  at  $> 99.998\%$  levels.

### III. Simulations

Using Duhamel's principle, the analytic solution to Fick's second law on a half-infinite line is

$$\phi(x, t) = KC_{out} - \int_0^t \text{erf}\left(\frac{x}{\sqrt{4D(t-\tau)}}\right) KC'_{out}(\tau) d\tau - KC_{out}(0) \text{erf}\left(\frac{x}{\sqrt{4Dt}}\right),$$

where  $K$  is the solubility of the material,  $D$  is the diffusion constant, and  $C_{out}$  is the outside concentration of the material. [?] For the out gassing process we are only able to detect the flux of material out of the plastic. This is given by Fick's first law evaluated at  $x = 0$ ,

$$J_{out}(t) = -K\sqrt{\frac{D}{\pi}} \left( \int_0^t \frac{C'_{out}(\tau)}{\sqrt{t-\tau}} d\tau + \frac{C_{out}(t)}{\sqrt{t}} \right),$$

where the sign has been flipped since the flux of material is outward. We see that it is no longer possible to evaluate  $K$  and  $D$  separately, since the diffusion in and out of the plastic is completely determined by the time-dependent concentration outside of the plastic. To simplify our model, we define a new constant

$$G = K\sqrt{\frac{D}{\pi}}.$$

We can fit the integral of our equation for the flux out of the plastic over time to out gassing data collected in Maryland's liquid xenon system to extract a

value for the constant  $G$ . With this method we constrain  $G \leq 0.01 \frac{\text{cm}}{\sqrt{\text{day}}}$ .

### A. Implications for LUX

With a constraint on  $G$  taken from the analytic solution to Fick's second law, we turn to numerical simulation to answer the question of how much initial  $\text{CH}_3\text{T}$  activity to inject into LUX to meet our calibration conditions. Several assumptions are made to simplify the numerical model. First, we approximate the diffusion into plastic as being a one dimensional process. Since the plastic in our detector at Maryland and in LUX can be approximated by a cylindrical shell, there is no dependence on the azimuthal or  $z$  coordinates. Since  $r$  is large compared to the thickness of the plastic shell,  $\frac{\delta^2 \phi}{\delta r^2} \gg \frac{1}{r} \frac{\delta \phi}{\delta r}$ , so Fick's laws in a one dimensional approximation become

$$J = -D \frac{\delta \phi}{\delta r} \vec{r}$$

$$\frac{\delta \phi}{\delta t} = D \frac{\delta^2 \phi}{\delta r^2}.$$

We assume the concentration of  $\text{CH}_3\text{T}$  in LUX is uniform throughout its volume, since the design of LUX creates currents which stir the liquid xenon. With perfect mixing the effect of the purifier can be modeled by adding an exponential time dependence to the outer volume. The time constant of this decay has an upper limit equal to the time it takes xenon to recirculate through the LUX detector, although in reality the mass transport from diffusion in the liquid and gaseous xenon decreases this time constant.

We use a simple implementation of the first order Euler method for our numerical simulations. The diffusion is simulated by setting the concentration at the boundary of the piece equal to  $KC_{out}$ , where  $C_{out}$  is

the concentration of  $\text{CH}_3\text{T}$  in the xenon. This concentration is dependent on time according to

$$\frac{\delta C_{out}}{\delta t} = J_{out} \frac{A_{plastic}}{V_{xenon}} - \frac{C_{out}}{\tau},$$

where  $A_{plastic}$  is the surface area of the plastic cylinder,  $V_{xenon}$  is the total volume of xenon in the fiducial region, and  $\tau$  is the time it takes for one full purification cycle. The first term on the right of this equation models out gassing of  $\text{CH}_3\text{T}$  from the plastic cylinder, while the second term models removal of  $\text{CH}_3\text{T}$  through purification. Using the first order Euler method, we arrive at an expression for  $C_{out}$  given by

$$C_{j+1} = C_j + \Delta t \left[ (J_{1,j} - J_{N_{x,j}}) \frac{A_{plastic}}{V_{xenon}} - \frac{C_j}{\tau} \right].$$

The initial concentration is defined by dividing the desired injection activity by the volume of the fiducial region. We choose  $D = 2.3 \times 10^{-9} \frac{\text{cm}^2}{\text{sec}}$  so that the half-infinite boundary conditions in our diffusion model is valid, and combine this with our allowed range of values for  $G$  to extract a value for  $K$ . We use this model to predict the total number of calibration events as well as the time required to return to  $<5\%$  of the nominal background rate for any  $\text{CH}_3\text{T}$  injection into LUX.

## IV. Experimental Setup

The setup of our tritiated methane calibration technique can be separated into three parts: the tritiated methane source bottle, the injection system, and the zirconium getter.

### A. The tritiated methane source

The tritiated methane source bottle for our calibration technique consists of a 2250 cc stainless steel bottle

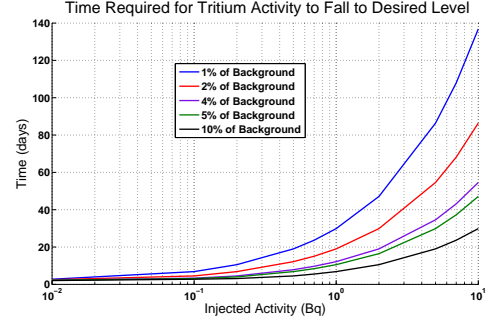


Figure 1: Time required to remove  $\text{CH}_3\text{T}$  from LUX after various injections.

which is filled with a mixture of tritiated methane and xenon. The purpose of this xenon is to serve as a carrier gas for the tritiated methane. The total activity in the source bottle is set by mixing a small amount of tritiated methane from a reservoir into the source bottle via volume sharing.

### B. The injection system

The injection system for our tritiated methane calibration technique consists of a series of expansion volumes which are used to fine tune the amount of  $\text{CH}_3\text{T}$  that is injected. Once the  $\text{CH}_3\text{T}$  source bottle is opened it flows through a methane gas purifier (SAES MC1-905F) to remove any sources of potential contamination, such as bare tritium. The  $\text{CH}_3\text{T}$  then flows into the expansion volumes set by the user. Once the expansion volumes have filled, the flow of xenon in the gas system is diverted through the expansion volumes to sweep the  $\text{CH}_3\text{T}$  into the detector. We continue to flow through the expansion volumes for one hour, which is equivalent to flushing out the expansion volumes over 1000 times, since LUX flows at 20 SLPM and the full 384.5 cc of the expansion volumes are filled with 1590 torr of the xenon and  $\text{CH}_3\text{T}$  mixture. A pump out port allows the expansion vol-

umes to be evacuated in preparation for each use of the injection system. Note that each injection will lower the total activity in the  $\text{CH}_3\text{T}$  source bottle via volume sharing, results in a smaller, yet calculable, injection activity with subsequent injections.

### C. The zirconium getter

The LUX gas system uses a hot zirconium getter (SAES-PS4MT15R1) downstream of the  $\text{CH}_3\text{T}$  injection system to remove  $\text{CH}_3\text{T}$  from the xenon. Extensive R&D was conducted using a smaller zirconium getter (SAES-PF4C3R1) at the University of Maryland to learn about the  $\text{CH}_3\text{T}$  removal efficiency of these purifiers. Details of these studies is discussed in section ??

## V. Injection Strategy

The LUX collaboration agreed upon a three phase plan for a safe and successful tritium injection. The first phase of this plan was a natural methane injection using the tritiated methane injection system for the purpose of determining the purification time constant in LUX. The second phase of the plan was a small tritium injection into LUX. This small injection would highlight any potential problems before injecting a larger amount of tritium, and it would determine if any scaling factor was needed between the absolute injection activity and the observed injection activity. Additionally, the small tritium injection would allow us to measure the fraction of tritium that goes into the fiducial volume. Finally, the third phase of the plan was to use what we learned from the first two phases to safely inject a larger amount of tritium for the purpose of measuring the ER rejection factor of LUX and cross-checking the NEST prediction of the ER band.

### A. Phase One

During phase one 0.02 grams of natural methane were injected into LUX using the tritium injection system. Purity samples from the detector were collected over the next few days, and a purification time constant of  $5.90 \pm 0.07$  hours was determined using data collected with the LUX gas sampling system.

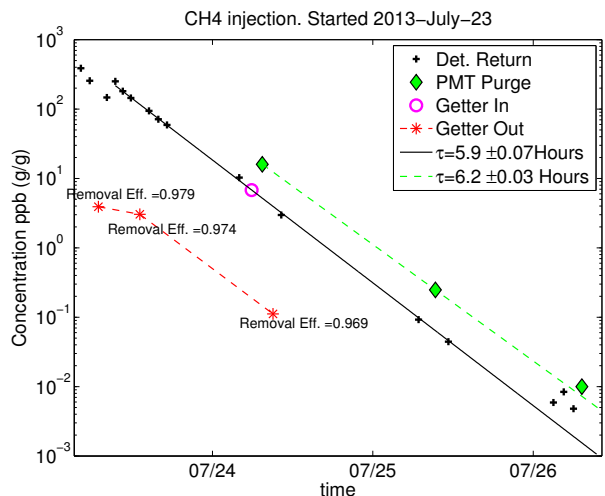


Figure 2: Removal of natural methane observed by the xenon sampling system prior to the tritiated methane injections.

### B. Phase Two and Three

The first, smaller tritiated methane injection on Aug-08-2013 was done to confirm the purification model established by a natural methane purification campaign the previous week. An absolute activity of 20 mBq of tritiated methane was injected, while actively purifying. A purification time constant of 6.7 hours was observed, consistent with the natural methane purification rate measured by the sampling system. After a day of circulating through the getter the tritium decay had fallen below detectable amounts confirming

the effective removal of the tritiated methane with the getter. On Aug-13-2013 a larger injection of 800 mBq was performed. The second injection produced 20,000 beta decay events in the LUX detector before being completely removed, 5000 of those events could be used to calibrate the ER band in the WIMP search region of 0-30 Phe (pulse area in photo electrons). Figure ?? shows the two tritium injections and the subsequent CH3T purification. Figure ?? shows the rate of events in the ER band before and after the tritium injection and removal. The CH3T was injected at the getter output but had passed through a special methane purifier to remove O<sub>2</sub> and H<sub>2</sub>O or other impurities that could cause a degradation in electron lifetime. The injections were performed with the getter in purify mode to maintain detector purity, as soon as the CH3T was injected it was immediately being removed. The rate of tritiated methane removal was consistent with the removal of natural methane observed by the xenon sampling system which was used to first verify the removal of methane to  $1/10^5$ . Figure ??.

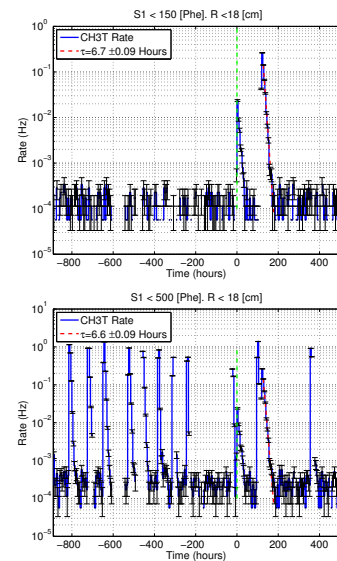


Figure 3: Left: Rate of events in the WIMP search region over a two month window. The dashed, vertical green line represents the time of the first tritiated methane injection. Right: The S1 threshold extended to 500 Phe to include rate spikes from the  $^{83}\text{Kr}$  injections, used for detector calibration during the science run.

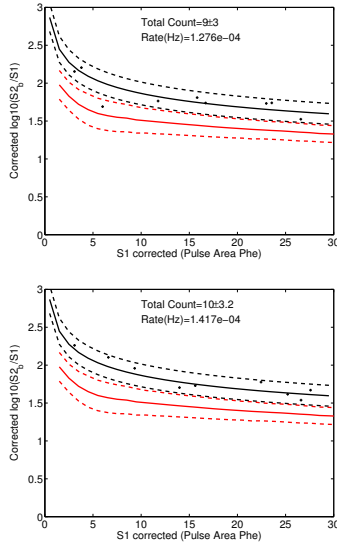


Figure 4: Left: 100 Hour time window in the WIMP search region before the tritiated methane injection. Right: 100 Hour time window in the WIMP search region after the purification of the tritiated methane.

## VI. Results from the Tritiated Methane Calibration

### A. Definition of Electronic Recoil Band and Comparison with NEST Model

The purpose of using the tritium calibration source was to get a handle on the electronic recoil (ER) band in the fiducial volume of the LUX detector. Separating ER and nuclear recoil (NR) events is crucial for background discrimination, unfortunately it is difficult to characterize low energy ER events with external calibration sources due to the self shielding properties of liquid xenon. Here we present the results of the ER band obtained from the beta decay of tritium, uniformly distributed, in comparison to the NEST simulation prediction at an extraction field of 120 V/cm. A key parameter obtained from the ER

and NR band is the leakage fraction which gives a rough measure of background rejection, for the current data set the NEST model along with AmBe and Cf neutron sources was used to define the NR band.

Leakage fraction is defined as the fraction of events in the ER band that spill into the lower half of the NR band. Tritium events are selected with standard WIMP search cuts using pulse classification, pulse pairing and the a quality cut. Two methods were used to calculate the leakage fraction. First, a cut and count in which the number of tritium events populating the lower half of the NR band are compared to the total number of tritium events in the selected S1 range. During the 24 hour acquisition of the tritium data used to define the ER band there was an expectation of just one event being non tritium, thus the cut and count method is valid in this case. The second method is to assume that the ER and NR bands are gaussian and calculate their overlap.  $(1 - \text{erf}((\text{Mean\_ER} - \text{Mean\_NR})/(\text{sqrt}(2) * \text{sigma\_ER}))))/2$ . Both methods yield good agreement which indicated that the distribution of ER events is mostly Gaussian. Figure ?? shows the leakage fraction per 2 Phe bins in S1. The mean leakage fraction from 0-30 Phe in the fiducial region is  $0.36\% \pm 0.01\%$ , see Figure ??.

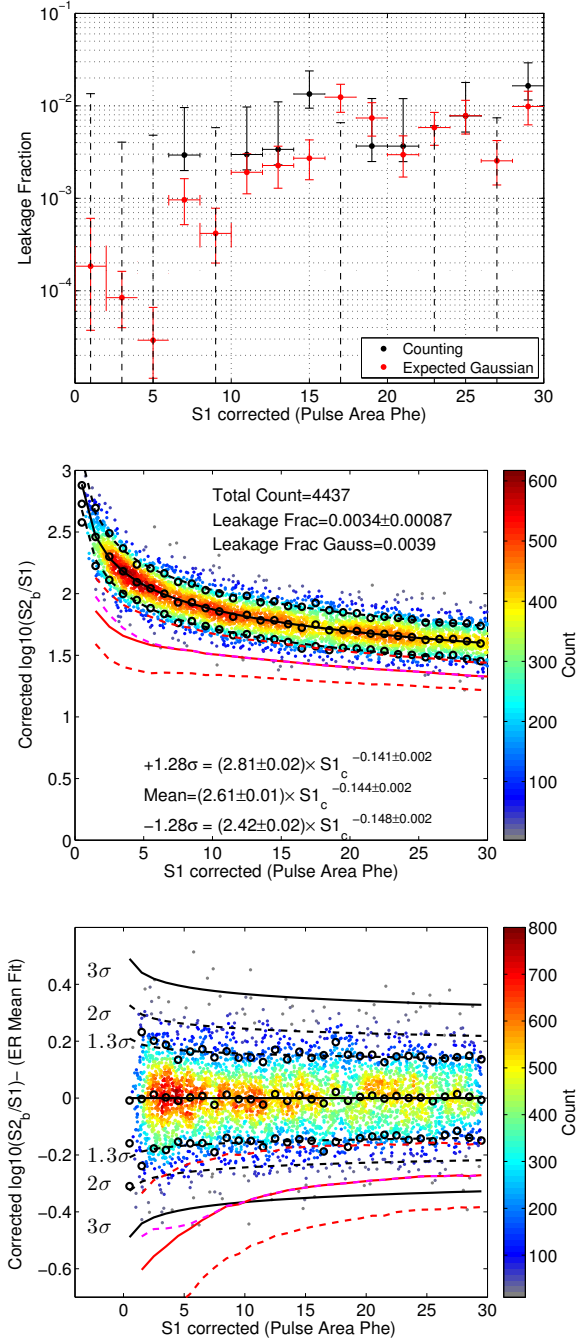


Figure 5: Top Left: Black, Leakage fraction calculated from cut and count. Red, leakage fraction expected from a Gaussian distribution. From 0 to 30 Phe with 2 Phe wide bins and not using the  $S2 > 200$  Phe cut. Top Right:  $\log(S2/S1)$  vs. S1 with ER band fit from the tritium data ( $S1$ : 0 to 30 Phe). Bottom. The data and fits renormalized to the ER band mean ( $S1$ : 0 to 30 Phe). The dashed magenta line is the NR mean with the  $S2 > 200$  Phe cut (using NEST 4-b for NR).

Figure ?? shows the comparison between simulation (NEST) and the data for the ER band. The agreement between simulation and data is good down to five phe in S1. At low energies, sub 2 keVee, the NEST model had not been vetted. The tritium data was ultimately used to define the ER band for the WIMP search run due to its high statistical significance. The newly acquired data was used to define a new NEST model that better reproduces the width and mean of the ER band at the extraction field of 120 V/cm.

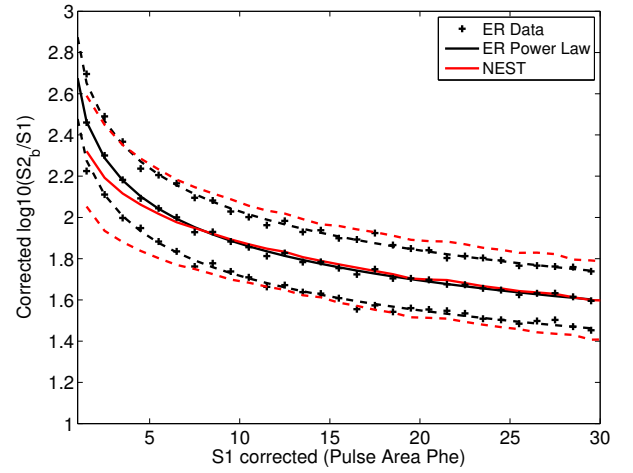


Figure 6: ER band from tritium data with  $\pm 1.3\sigma$  (black) compared with NEST simulation prediction (Red).

## B. Distribution of Tritiated Methane

Tritium events appear uniformly distributed in the detector thirty minutes after the tritiated methane injection. Figure ?? shows the Z, XY and radial distribution of tritium events after an injection. When considering the tritium events a drift time cut from 5 to  $324 \mu s$  was made to cover only the region from the gate to the cathode, excluding the region between the gate and anode. An additional cut requiring that the



event be between  $\pm 2\sigma$  of the ER mean was made to minimize the leakage of residual alphas from the walls and cathode. The tritiated methane quickly dispersed throughout the liquid decaying in all regions on the detector, proving to be an ideal low energy calibration source.

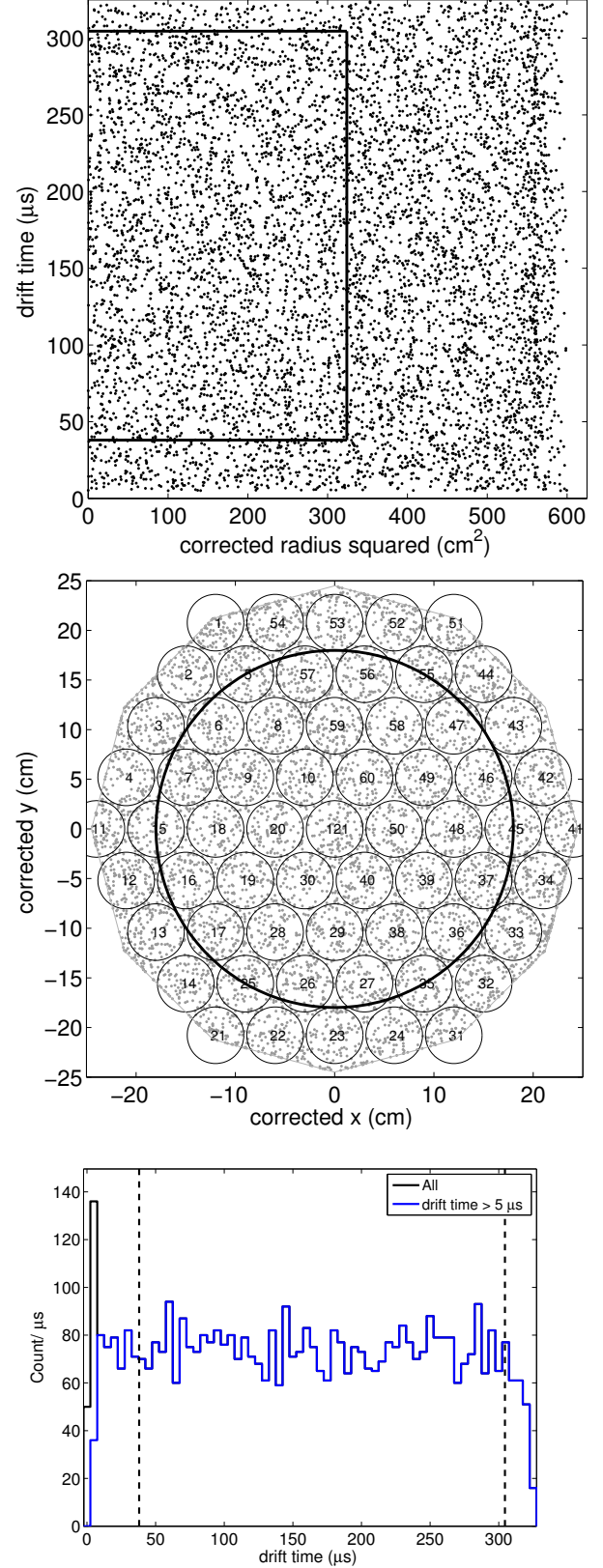


Figure 7: Top Left: The distribution of tritium events vs. corrected radius squared. Top Right: The distribution of tritium events vs. XY-corrected in the region between the gate and the cathode, as reconstructed by the Mercury algorithm (used for LUX po-

### C. Combined Energy Calibration

To transform S1\_Phe and S2\_Phe to absolute energy we use a model that uses the number of quanta produced as its input, Ref[1].  $E(s1, s2) = S1/PDE * S2/(extractioneff * single - electron - size)$ . The single electron size was calculated to be 10.57 Phe, the extraction efficiency for elections was calculated to be 0.65 and the photon detection efficiency (PDE) was calculated to be 0.14.

The agreement between that data and SIM indicate that we have a good understanding of our absolute energy scale down to 2 keV<sub>ee</sub>. Between 1 and 2 keV<sub>ee</sub> there is a region with excess events, this is likely an indication that the model used for determining energies is breaking down and needs further investigation.

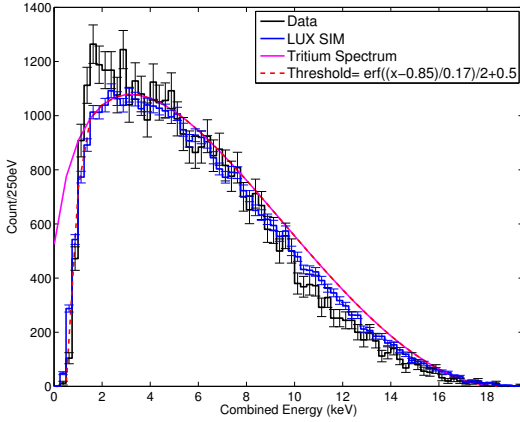


Figure 8: Combined energy spectrum of the Data, LUX SIM and Raw NEST model for tritium beta decay. Note, Raw NEST is with photon and electron propagation turned off which represents the tritium beta spectrum before smearing due to detector resolution.

### D. Absolute Rate

The absolute efficiency for detecting tritium events can be determined by comparing the number of observed events to the number expected. The initial activity injected was calculated to be  $0.84 \pm 0.22$  Bq, with the largest uncertainty coming from the ratio of  $CH_3T/CH_4$  from the tritiated methane source bottle. The purification time constant was measured to be 6.6 hours. From the initial rate and the purification constant we expect to count a total of  $20,200 \pm 4,000$  events in the LUX detector before applying the S1 threshold. With the S1 threshold we expect  $16,000 \pm 3,100$  ‘golden’ events. The actual count observed in the liquid xenon volume was 20,000 events, which is in good agreement with the expected value taking into account the uncertainty in the initial activity and the purification model. After making fiducial cut  $7,700 \pm 1,500$  events were expected, roughly  $16,000 \pm 3,100 * (290/324) * (18^2/24.5^2)$ . And a total of  $9,500 \pm 100$  were observed, see Figure ??.

### E. Data vs. SIM

The SIM contained a total of 200,000 tritium events but after WIMP search cuts there remained 156,000 due to the S1 threshold. The overall scaling between the LUX\_SIM and the Data was expected to be 156,000 events total in SIM and 20,000 in Data (for golden events), this corresponds to a factor of 1/7.8 for Data/Sim. The best fit to the S2 spectrum was found to be 1/7.9 and the best fit to the energy spectrum was found to be 1/7.5, both in good agreement with the expected rate.

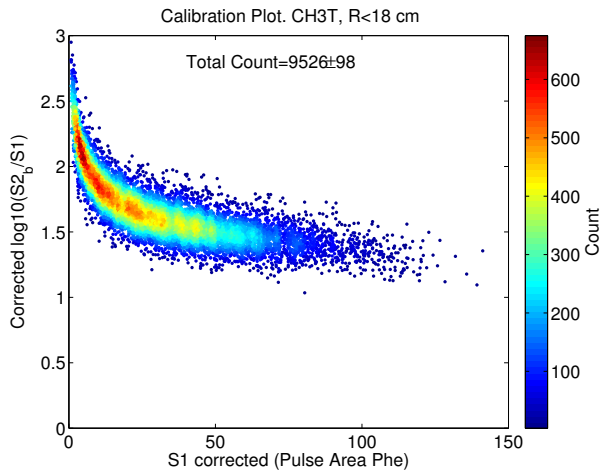


Figure 9: Combined energy spectrum of the Data, LUX SIM and Raw NEST model for tritium beta decay.

## VII. Summary

We have presented our new technique for injecting and removing  $\text{CH}_3\text{T}$  as an internal calibration source in detectors which utilize liquid and gas phase noble gases. We discussed the assembly of our  $\text{CH}_3\text{T}$  calibration system, motivated by gas and liquid phase R&D experiments at the University of Maryland. We have used data from the LUX detector to show that our system can safely inject  $\text{CH}_3\text{T}$  for the purpose of internal calibration.

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