

Characterizing the Peripheral Dynamics of Xenon Dark Matter Detectors

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*To my parents, who supported and encouraged me from my earliest years
and to my wife Linda, for always being there to help me find the way*

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Abstract

One of the most important fundamental problems in physics today is to understand the nature of dark matter. The landscape of explanations for observed dark matter phenomena is vast and still expanding, and an impressive number of experiments have been built to probe the dark sector of the universe.

A prominent class of detectors is aimed at discovering (or excluding) a particular kind of dark matter: the Weakly Interacting Massive Particle (WIMP). Searching for this popular dark matter candidate requires an ultra-sensitive, low-background target; xenon detectors serve as such a target for dark matter interactions.

The Large Underground Xenon (LUX) detector is a dual-phase xenon time-projection chamber (TPC) which was operated underground at the Homestake Mine in Lead, South Dakota from 2013 to 2016, and was able to achieve the world’s leading WIMP exclusion limit. However, successful reconstruction of WIMP-nucleus scatters in such detectors requires thorough understanding of the detection medium, which is made difficult by various confounding effects near the detector walls. Field-fringing is a major component of confusion in the periphery, and the large electric field non-uniformities in Run 4 of LUX provided a significant challenge in the dark matter analysis. Here is presented an algorithm to bijectively map between reconstructed event positions and true spatial coordinates, which serves as an important tool for studying field effects and fiducialization in LUX.

Additionally, a successful dark matter search must model interfering background events in the WIMP search region which can’t be directly vetoed. One class of unavoidable backgrounds comes from nuclear decay chain daughters in detector materials themselves, which may produce WIMP-like signals (an effect which is amplified due to various detector effects). The Davis Xenon (DAX) test bed system and a dual-phase TPC have been assembled and operated at UC Davis to characterize these common “wall backgrounds”, as well as perform other R&D studies for the next-generation LUX-ZEPLIN (LZ) experiment. The DAX TPC specifically measures the xenon response to heavy nuclei produced by custom α decay sources created using novel chemical deposition procedures.

In this thesis, results will be presented for the light and charge yields of immersed localized sources of ^{206}Pb ions in liquid xenon, as well as a method for tagging such recoil events *in situ* by using PIN diodes as charged particle detectors to capture the correlated α particles. We also compare our isolated ^{206}Pb events with previous WIMP search data from LUX, and discuss the significance of ^{206}Pb as a WIMP background.

Such information is most useful to future experiments if it can improve existing background models and simulations. The Noble Element Simulation Technique (NEST) is the ultimate software package for calculating expected signal yields in xenon detectors, but is an empirical framework that relies on experimental data to inform the models. We discuss the development of current NEST v2 models, specifically the heavy nuclear recoil models, as well as our current understanding of the xenon microphysics. We also show NEST predictions for mono-energetic ^{206}Pb recoils, and discuss how our most recent DAX ^{206}Pb measurements may inform NEST models in future work.

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My parents nurtured my love to read from an early age, tolerated my “insatiable curiosity” (as my grade school teacher put it), and encouraged me to pursue my passions to the fullest, whether that was creative writing, music, or particle physics. They taught me work ethic, perseverance, healthy skepticism, and simply how to be the best person I can be.

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Chapter 1

Dark Matter

“I have approximate answers and possible beliefs, and different degrees of certainty about different things...but I’m not absolutely sure of anything, and there are many things I don’t know anything about!”

— Richard Feynman

For decades, physicists have predicted and confirmed the existence of numerous particles which make up our universe. Our attention may well have been diverted almost exclusively to theories of quantum gravity and grand unification, were it not for a curveball thrown by nature (as it tends to do). While particle physicists were validating the Standard Model with extraordinary precision, astronomers were detecting anomalous clouds in distant galaxies. For the better part of a century, evidence has been mounting that we in fact do not understand the primary component of matter in our universe.

The partitioning of energy density in the universe is now rather well-constrained [225]. Dark energy, which drives the accelerated expansion of the universe, comprises the majority of the energy density at $\approx 69\%$. Only $\approx 5\%$ is from baryonic matter. The remaining 26% is an additional form of matter which is implicated by its observed gravitational effects, but whose particle constituents are not known.

Many have attempted to explain away this so-called “dark matter” by offering tunings and modifications of already established cosmological models. However, it has become increasingly clear over the last few decades that particulate models of dark matter provide an

enticing posterior explanation of the observed universe.

Dark matter is not an answer. It remains one of the universe’s deepest scientific mysteries, and is really just a name which encompasses an enormous range of possible theories. Physicists continue to constrain phase space from a variety of experimental angles, but the matter remains dark. Even the most well-motivated candidates have eluded detection, but our attempts to capture the essence of dark matter will hopefully encourage creativity to the point of revelation.

1.1 Cosmological Motivations

1.1.1 Quantifying the Luminous Matter

While terminology such as “dark matter” or “dark bodies” dates back to the works of Kelvin, Poincare, and Opik in the early 1900s, the first claims for an excess of dark matter (using dynamical evidence) came from a Swiss astronomer named Fritz Zwicky [62].

While working at the California Institute of Technology in 1933, Zwicky was studying the dynamics of galaxy clusters and came to an interesting conclusion. Using the velocity measurements of eight galaxies in the Coma cluster measured by Hubble and Humason [128], Zwicky deduced that the mass was much greater than expected given the observed luminosities. In a refined analysis in 1937, Zwicky demonstrated perhaps the first use of the Virial Theorem to estimate the mass of a galaxy cluster [247].

The Virial Theorem can be applied as follows. For a central force acting on the k th body of a system of n objects, we can expand the force law using the chain rule:

$$\begin{aligned}\vec{F}_k &= m_k \frac{d^2 \vec{r}_k}{dt^2} \\ \implies \vec{r}_k \cdot \vec{F}_k &= \frac{1}{2} \frac{d^2}{dt^2} (m_k r_k^2) - m_k \left(\frac{d\vec{r}_k}{dt} \right)^2\end{aligned}\tag{1.1.1}$$

For gravitational forces that take the form of Newton’s inverse square law, summing over k gives (with moment of inertia I , kinetic energy K , and potential energy U):

$$U = \frac{1}{2} \frac{d^2 I}{dt^2} - 2K$$

Assuming a stationary system, or one that is in statistical equilibrium, the moment of inertia fluctuates around some mean value and its derivatives vanish when time-averaged, giving

$$\langle U \rangle = -2 \langle K \rangle \quad (1.1.2)$$

In a self-gravitating system, the gravitational potential energy can be obtained by integrating over shells of mass dm at radius r' interacting with the mass contained, $M(r')$:

$$M(r) \langle v^2 \rangle = \int_0^r \frac{G M(r')}{r'} dm \quad (1.1.3)$$

where $\langle v^2 \rangle$ is the mean square velocity of the mass distribution. Assuming a spherically symmetric mass density of the form a/r^m (with $m \neq 3$),

$$M(r) = \int_0^r \frac{a}{r'^m} 4\pi r'^2 dr' = \frac{4\pi a}{3-m} r^{3-m} \quad (1.1.4)$$

Inserting $M(r')$ into Eq. 1.1.3 and performing some algebraic manipulation gives a useful relationship between the mass and mean square velocity:

$$M(r) = \left(\frac{5-2m}{3-m} \right) \frac{\langle v^2 \rangle r}{G} = \frac{\kappa \langle v^2 \rangle r}{G} \quad (1.1.5)$$

where $m \neq 3$. Note that $\kappa = 1$ for the famous isothermal profile $\rho \propto 1/r^2$ (where $m = 2$).

For astronomers, the velocity dispersion σ_v is measured from the width of spectral lines and serves as an estimator for the RMS velocity, i.e. $\sigma_v \approx \sqrt{\langle v^2 \rangle}$. If velocity isotropy is assumed, the dispersion in the tangential components of the velocity is equal to that of the radial (or line-of-sight) component, implying that $\langle v^2 \rangle = \sigma_v^2 = \sigma_r^2 + \sigma_{t1}^2 + \sigma_{t2}^2 = 3\sigma_r^2$, where σ_r denotes the radial velocity dispersion measured from redshifts.

Assuming a constant mass density ($m = 0$) and velocity isotropy, Eq. 1.1.5 becomes

$$M(r) = \frac{5 \langle v^2 \rangle r}{3G} = \frac{5 \sigma_r^2 r}{G} \quad (1.1.6)$$

Using such a formulation of the Virial Theorem, along with some conservative assumptions about the radial distribution of the matter, Zwicky estimated an average galactic mass of 4.5×10^{10} solar masses in the Coma cluster, giving a mass-to-light ratio of $\gamma = 500$ [247]. This deviates by a huge factor from the expected $\gamma \sim 3$, implying an enormous excess of mass. We now know that this number was highly inflated for multiple reasons:

1. An incorrect Hubble parameter was being used at this time, heavily altering the expected mass-to-light ratio. This reduces the excess by a factor of ≈ 8 [62].
2. Zwicky did not have X-ray imaging at his disposal, and so could not take into account the spectrum of hot X-ray emitting gas.

The discovery of this hot gas marked the next phase of precision in quantifying the matter in galaxy clusters, however this did not follow until decades after Zwicky’s claim. With technological advancements in X-ray telescopes, specifically grazing incidence optics, it became possible to map this additional mass component.

In 1963, Arrigo Finzi considered the possibility that hot gas comprises some of the “missing” matter in galaxy clusters, and theorized that the gas would have a temperature giving a velocity dispersion comparable to that of the galaxies (≈ 1000 km/s) [199]. This would also imply that the gas undergoes thermal emission via bremsstrahlung. Finzi also prudently claimed that the gas could not be the binding mass of the clusters, since the gas would cool on timescales far shorter than that needed for structure formation.

After the discovery of X-ray emission from galaxy clusters in the early 1970s, the X-ray spectra were characterized over a range of temperatures. The intensity spectrum followed an exponential distribution, indicating a thermal emission process:

$$I(E) \sim e^{-h\nu/kT} \tag{1.1.7}$$

where $h\nu$ is the radiation energy. Using this model for thermal emission, one can find the temperature of the gas by fitting the intensity spectrum as a function of energy, then determining the 3-dimensional density distribution from the intensity map.

The mass distribution of the gas can be estimated with the assumption that it is in hydrostatic equilibrium (i.e. gravitational forces are balanced by ordinary gas pressure). If we take an isothermal gas to be ideal and have a spherically symmetric density, we can balance forces on an infinitesimal element:

$$-A dP - \frac{GM(r) dm}{r^2} = \rho A dr \frac{d^2r}{dt^2} = 0$$

Here, A is the area of the element, dP is the differential pressure, dm is the mass of the element, and the last equality just uses that $F = dm \cdot a = 0$. Manipulation gives

$$\frac{dP}{dr} = -\frac{GM(r)\rho}{r^2}$$

The ideal gas law, $PV = NkT$, gives

$$P = \frac{NkT}{V} = \frac{kT}{\mu m_p} \frac{M}{V} = \frac{kT}{\mu m_p} \rho \implies \frac{dP}{dr} = \frac{k}{\mu m_p} \frac{d}{dr}(T\rho)$$

where μ is the mean atomic weight, m_p is the mass of a proton (hydrogen), T is the temperature of the isothermal gas, and ρ is the mean gas density. Combining the two equations, we can calculate the distribution of gravitating mass:

$$M(r) = -\frac{kTr^2}{\mu m_p G} \left(\frac{1}{\rho} \frac{d\rho}{dr} + \frac{1}{T} \frac{dT}{dr} \right) \quad (1.1.8)$$

If temperature is constant in radius, further manipulation gives

$$M(r) = -\frac{kTr}{\mu m_p G} \left(\frac{d(\ln \rho)}{d(\ln r)} \right) \quad (1.1.9)$$

X-ray measurements of the M87 galaxy in 1980, made using the Einstein Observatory, yielded a mass of $\sim 10^{13}$ solar masses whose distribution extended far beyond the visible core [95]. Further analyses in the 1980s reinforced this claim, that the gas content in galaxies exceeded the mass of the stars by a factor of ~ 4 . However, in the outermost reaches of galaxy clusters, the dynamical mass ranges upward such that there is still 5–6 times more mass than accounted for by the luminous matter [199]. Zwicky’s numbers may have been overblown, but he had actually stumbled upon multiple invisible mass components.

1.1.2 Galactic Rotation Curves

Another discovery which led to serious consideration of the dark matter hypothesis was the observation of anomalous galactic rotation. These precise measurements began to convince the community that something was indeed wrong with models of galactic composition.

The surface brightness for galaxies with a disk-like profile (beyond the central bulge component) has the functional form [103]:

$$\Sigma = \Sigma_0 e^{-r/h} \quad (1.1.10)$$

where h is known as a “scale length”. It is clear from this profile that the luminous stellar and gaseous matter is almost completely contained within a few scale lengths. Beyond this point, there should be a Keplerian decline in the measured orbital velocity of the galaxy. From Newtonian gravity, the orbital velocity of a mass distribution is given by

$$\frac{v^2(r)}{r} = \frac{GM(r)}{r^2} \implies v(r) = \sqrt{\frac{GM(r)}{r}} \quad (1.1.11)$$

If the majority of mass is contained within radius r , we expect the velocity to go like $1/\sqrt{r}$.

While teaching a graduate course in astronomy at Georgetown University in 1962, Vera Rubin published a paper with her students in which they derived a rotation curve for a catalogue of early-type stars in the Milky Way. They found that “for $R > 8.5$ kpc, the stellar curve is flat, and does not decrease as is expected for Keplerian orbits” [191]. This was met with some negative and unpleasant feedback from the scientific community [193].

In the 1970s, Rubin and her colleague Kent Ford used a state-of-the-art spectrograph to study the Andromeda Galaxy (M31) in the optical spectrum. In such gas-rich spiral galaxies, young stars emit UV radiation which ionizes the surrounding hydrogen gas, creating continuous visible HII lines from recombining hydrogen; doppler shifts in these emission lines then allow for the derivation of orbital velocities as a function of radial distance. Their measurements yielded a flat rotation curve out to 24 kpc [194].

While their work showed early tantalizing hints, it was neither claimed nor demonstrated at this point that dark matter halos were necessary. It was still possible to construct disk mass profiles which fit well to data out to a few scale lengths, since the velocity falloff is rather slow [30, 62]. It was perhaps Ken Freeman who made the first unambiguous claim of a mass discrepancy. In 1970, he combined theoretical modeling with radio observations to conclude that the distributions of undetected mass in NGC 300 and M33 would deviate significantly from the optical component [103].

Advancements in radio astronomy were needed to make claims about the outermost regions of galactic mass distributions, since ionized hydrogen exists only in very faint components at large radii. Neutral hydrogen, which constitutes a small mass fraction and extends well beyond the optical radius, serves as an ideal tracer of the rotational velocity (yielding rotation curves $\sim 50\%$ further out than optical measurements [193]). In the 1970s, 21-cm line receivers became available for radio telescopes, allowing for the measurement of this hydrogen. The 21-cm line (1420 MHz) comes from the hyperfine transition of the hydrogen atom’s spin from parallel to antiparallel through a magnetic spin interaction. Furthermore, hydrogen is abundant and HI is not impeded by interstellar dust, giving strong lines [199].

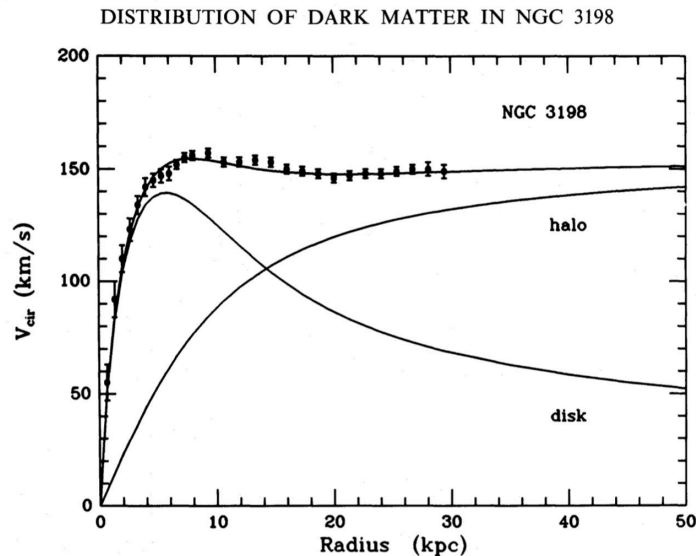


Figure 1.1: The orbital velocity of galaxy NGC 3198 as a function of radius. Also shown are the best-fit disk and halo mass components.

As can be seen from Fig. 1.1, measurements using the 21-cm line gave a very precise rotation curve out to 30 kiloparsecs. It is clear that a “dark halo” mass component is necessitated to produce an accurate fit [30]. We see from Eq. 1.1.11 that to obtain a flat rotation curve, i.e. $v(r)$ is constant, we require that $M(r) \sim r$. It follows that for a spherically symmetric mass distribution $\rho(r)$,

$$v(r) = \sqrt{\frac{4\pi G}{r} \int_0^r \rho(r') r'^2 dr'} \quad (1.1.12)$$

which implies an asymptotically isothermal mass density profile, $\rho(r) \sim 1/r^2$.

Precise radio measurements by Roberts and Rots in 1973 [186] and Roberts and Whitehurst in 1975 [238][185] laid a convincing case for dark halos and the necessary modification of mass-to-light ratios. Rubin and Ford proceeded to investigate a large number of spiral galaxies using extended optical measurements, and their findings further supported these flat rotation curves [192].

1.1.3 Cosmological Structure Formation

More indirect evidence for dark matter emerged from early-universe cosmological models. Matter distribution in the early universe determined the gravitational structure formation leading to the “clumpiness” we observe today on large scales, so studying the evolution of density variations provides hints about the matter distribution of the past.

The cosmic microwave background (CMB) provides a significant amount of information regarding the historical evolution of our universe. The CMB is the black body spectrum of microwave radiation detected at redshift $z \sim 1100$, and has a temperature of 2.75 K [136]. It is also known as the “surface of last scattering”, since it represents the transition where the hot ionized gas in the universe became transparent to photons, which were emitted at visible and UV wavelengths and are observed after being redshifted down to microwave range.

Let us consider Newtonian density perturbations in a baryon-photon fluid of the early universe. We consider such a fluid expanding due to “Hubble flow” in the hot, dense early universe, before the decoupling of photons from the baryonic matter. This flow is governed by a time-dependent Hubble parameter $H(t)$. Linear perturbations to the fluid are given by:

$$\begin{aligned}\rho &\rightarrow \bar{\rho}(t)(1 + \delta), & P &\rightarrow \bar{P}(t) + \delta P \\ \vec{u} &\rightarrow a(t)H(t)\vec{x} + \vec{v}, & \Phi &\rightarrow \bar{\Phi}(\vec{x}, t) + \phi\end{aligned}$$

where δ is the density perturbation of the mean $\bar{\rho}$, δP and ϕ are departures from the mean pressure and gravitational potential respectively, $a(t)$ is a cosmological scale factor used to define comoving distance scales, and $\vec{v}$ is the departure of the fluid velocity from the

background Hubble flow (the peculiar velocity).

We also need the relevant equations describing the dynamics of a gravitational fluid [173]:

$$\text{(Continuity)} \quad \partial_t \rho + \nabla_t \cdot (\rho \vec{u}) = 0$$

$$\text{(Euler)} \quad \partial_t \vec{u} + \vec{u} \cdot \nabla_r \vec{u} = -\frac{1}{\rho} \nabla_r P - \nabla_r \Phi$$

$$\text{(Poisson)} \quad \nabla_r^2 \Phi = 4\pi G \rho$$

A common approximation used by cosmologists is to assume a barotropic fluid; this means that the pressure P is a function of the density ρ only, which gives a direct proportionality between the density and pressure perturbations:

$$\delta P = \frac{\partial P}{\partial \rho} \bar{\rho} \delta = c_s^2 \bar{\rho} \delta$$

Here, c_s is defined to be the propagation speed of sound waves in the medium.

Taking the time derivative of the continuity equation and doing some algebraic manipulation yields the differential equation for fluid dynamics in an expanding universe [173]:

$$\partial_t^2 \delta + 2H \partial_t \delta + \left(\frac{c_s^2 k^2}{a^2} - 4\pi G \bar{\rho} \right) \delta = 0 \quad (1.1.13)$$

The critical value which gives oscillatory solutions for this equation defines a minimum distance scale over which sound waves must travel in order for gravity to counteract the pressure resisting collapse. This was discovered by Sir Jeans in 1902, and is known as the Jeans wavelength:

$$\lambda_J \equiv \frac{2\pi a}{k} = \sqrt{\frac{\pi c_s^2}{G \bar{\rho}}} \quad (1.1.14)$$

We can see that if the density perturbation δ is decomposed into Fourier modes, the Jeans length determines which modes are oscillating and which are growing. It is common to see a power spectrum defined by such perturbation modes,

$$P(\vec{k}) \equiv |\delta_k(\vec{k})|^2 = \left| \int \delta(\vec{x}, t) e^{-i\vec{k} \cdot \vec{x}} d^3x \right|^2 \quad (1.1.15)$$

These perturbations are not static; they evolve with the universe. There are multiple epochs leading up to decoupling: the radiation-dominated era (RDE) and the matter-dominated era (MDE). There are different perturbation growth laws in each era, since the growth of perturbations depends on the pressure support provided by baryonic coupling.

The “horizon”, the causally connected region of spacetime defined by the Hubble parameter at redshift z by $1/H(z)$, is an important concept that also determines which modes influence structure. Fluctuations with $\lambda > 1/H$ are considered “super-horizon”, whereas fluctuations with $\lambda < 1/H$ are “sub-horizon”. Super-horizon modes must be treated with general relativity and are outside the scope of these Newtonian arguments. Suffice it to say that while these super-horizon fluctuations may grow by the same power laws as sub-horizon fluctuations, they will only result in density perturbations once they enter the horizon due to the expansion of the horizon itself [136].

During RDE, sub-horizon fluctuations smaller than the Jeans length simply oscillate in the baryon-photon fluid, while larger sub-horizon modes would grow as

$$\delta \sim a^2 = \frac{1}{(1+z)^{-2}} \quad (1.1.16)$$

since they resist the pressure from baryonic coupling. During MDE, there is no pressure support and all sub-horizon modes grow together as

$$\delta \sim a = \frac{1}{1+z} \quad (1.1.17)$$

The photon-baryon fluid before recombination has a Jeans length on the order of the horizon size, meaning that sub-horizon fluctuations do not grow, but simply fluctuate. At decoupling, a dramatic pressure drop decreases the Jeans length and baryonic masses begin collapsing on sub-horizon scales. Therefore, the CMB should provide a perfect snapshot of perturbations in the baryon-photon fluid before the density contrast could grow.

By relating the measured temperature anisotropies of the CMB to density fluctuations, we can compare with the predicted density variations at decoupling. To produce the presently observed structure, we would need $\delta \sim 10^{-4}$, corresponding to comparable fluctuations over

arc minutes in the CMB [199]. However, as early as the 1980s, fluctuations on this scale were not observed, leading to concerns about the model of a lone baryon-photon fluid.

If we propose an additional fluid which is decoupled from the baryon-photon fluid with a Jeans length of effectively zero, its density fluctuations would grow on all scales. This component would begin collapsing during MDE but *before* decoupling, forming gravitational potential wells for the baryonic matter to fall into *after* decoupling. Such structure formation gives a strong argument for cold dark matter, and is further discussed in Sec. 1.2.5.

1.1.4 Gravitational Lensing and the Bullet Cluster

More recent and irrefutable evidence for dark matter emerged with the usage of gravitational lensing to map out mass distributions of galaxy clusters. Gravitational lensing is an important and powerful tool that measures effects predicted by Einstein’s theory of general relativity. We start with Einstein’s equation:

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = 8\pi G T_{\mu\nu} \quad (1.1.18)$$

This non-linear tensor equation relates the geometry of spacetime on the left hand side, completely determined by the metric tensor $g_{\mu\nu}$, with the dynamics of matter represented by the energy-momentum tensor $T_{\mu\nu}$ on the right hand side [73].

This equation predicts that light follows null geodesics, meaning the spacetime interval vanishes ($ds = 0$), so the curvature of spacetime causes deflects light by a precise factor that depends on the mass distribution of the “lensing” object. For many cases of astrophysical interest, it is sufficient to assume a “weak lens”, or one whose gravitational potential $\Phi \ll c^2$ [160]. In such a case, the metric $g_{\mu\nu}$ which describes the geodesics of spacetime is a simple perturbation of the Minkowski metric $\eta_{\mu\nu}$ (the metric for flat spacetime):

$$\eta_{\mu\nu} \rightarrow g_{\mu\nu} = \eta_{\mu\nu} + I \left(\frac{2\Phi}{c^2} \right)$$

This metric gives the spacetime interval

$$ds^2 = \left(1 + \frac{2\Phi}{c^2} \right) c^2 dt^2 - \left(1 - \frac{2\Phi}{c^2} \right) (d\vec{x})^2 \quad (1.1.19)$$

Take a mass concentration at redshift z_L and angular diameter distance D_L , acting as a lens on the light source at z_S with angular diameter distance D_S . Relative to the optical axis, the source at angular position $\vec{\beta}$ and position βD_S causes a light ray having impact parameter $\vec{\xi} = \vec{\theta} D_L$ to have the following apparent deflection angle:

$$\vec{\alpha} = \frac{D_{LS}}{D_S} \frac{2}{c^2} \int_{-\infty}^{\infty} \vec{\nabla}_{\perp} \Phi \, dz$$

In the case of “strong” gravitational lensing, such deflections of light actually may actually form multiple complete images of the source, or even smear the light into an Einstein ring. In the case of “weak lensing”, where the light from background source galaxies is only weakly distorted by a lensing galaxy cluster, we may introduce a lensing potential ψ obtained by projecting and rescaling the Newtonian potential Φ [180]:

$$\psi(\vec{\theta}) = \frac{D_{LS}}{D_L D_S} \frac{2}{c^2} \int \Phi(D_L \vec{\theta}, z) \, dz \quad (1.1.20)$$

Derivatives of this potential give the deflection angle $\vec{\alpha}$ and “convergence” κ :

$$\vec{\nabla}_{\theta} \psi = \vec{\alpha}, \quad \nabla_{\theta}^2 \psi = \frac{2}{c^2} \frac{D_L D_{LS}}{D_S} 4\pi G \Sigma = 2 \kappa(\theta) \quad (1.1.21)$$

Here, Σ is the surface mass density of the lens.

The distortion of the source image can be described to first order by the Jacobian matrix:

$$A \equiv \left(\delta_{ij} - \frac{\partial^2 \psi(\vec{\theta})}{\partial \theta_i \partial \theta_j} \right) = (1 - \kappa) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \gamma \begin{pmatrix} \cos 2\phi & \sin 2\phi \\ \sin 2\phi & -\cos 2\phi \end{pmatrix} \quad (1.1.22)$$

The angle ϕ anti-symmetrizes the “shear” component (the right term), and the left term is the “convergence” component. This shows that while the convergence isotropically scales the source image, the shear warps the shape along a specific direction (determined by the lensing potential). Thus, a circular source becomes an ellipse.

While precisely measuring the elliptical distortions of single galaxies is difficult, a statistical analysis of many background objects allows for the detection of coherent distortions due to a lensing mass. The second moment of surface brightness profiles can be used to

measure ellipticity, which is then corrected for anisotropies and instrumental smearing [77]. The overall corrected ellipticity is then a measure of the “reduced shear”:

$$\vec{g} = \frac{\vec{\gamma}}{1 - \kappa} \quad (1.1.23)$$

The shear allows us to infer the lensing potential, and therefore the convergence and mass density of the foreground lensing object.

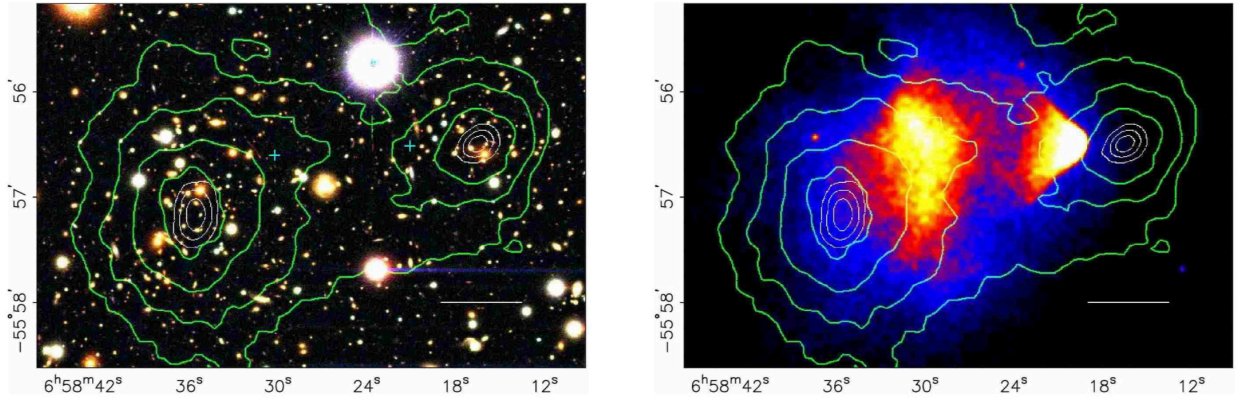


Figure 1.2: The Bullet Cluster merger. The green contours represent the mass distribution measured from lensing, which is overlaid on the visible image (left) and on color maps of the X-ray emitting gas (right) [77].

A very important use of this lensing technique was in the analysis of the Bullet Cluster merger (see Fig. 1.2), where two galaxy clusters have rammed through each other. The stellar content has passed through unheeded, since these bodies only interact feebly via gravitational forces and are sparse. However, the intra-cluster medium (ICM), the hot gas comprising the majority of baryonic mass, becomes a shock wave-forming plasma when passing through another cluster at supersonic speed.

The two clusters collided at ≈ 4700 km/s, causing the plasma fluid to experience ram pressure, forming a shock wave front. X-rays are produced from fast clouds of hot gas coming together, the ions scattering off each other and decelerating, causing X-ray radiation through bremsstrahlung [70, 77]. The X-ray spectrum gives the temperature and allows for a 3D cluster model of the plasma mass distribution. Since the gas is the majority of luminous

mass, we would expect that the centers of mass should lie near the centers of the two gas regions.

Weak gravitational lensing, which traces the absolute mass distributions of the clusters, shows that the centers of mass are actually displaced from the majority of the luminous mass. This implies that a large component of non-luminous matter must be present. Since this matter passed through the merger unheeded, an upper limit can be placed on the self-interaction cross-section [187]. This is essentially a “smoking gun” for dark matter, since it does not rely on questionable assumptions of symmetry or hydrostatic equilibrium [77].

1.2 The Landscape of Explanations

The evidence for dark matter is as varied as it is abundant, and thus its existence is difficult to refute. Each of the anomalies described above is a puzzle piece, and they only seem to fit neatly within the frame of the dark matter hypothesis. Below we will discuss some theories which seek to explain these phenomena, both DM and non-DM.

1.2.1 MACHOs

It has been theorized that the excess mass observed in galactic halos may be composed of yet-undetected baryonic bodies such as brown dwarfs, black holes, or other stellar remnants. However, measuring the contribution of such bodies (called Massive Compact Halo Objects, or MACHOs) to the overall halo mass is non-trivial.

The discovery that gravitational microlensing may be the key to quantifying such bodies is often attributed to Paczyński [170]. Microlensing is the special case of gravitational lensing in which a light source is split into unresolvable images, causing a time-dependent amplification of the apparent brightness due to relative motions of the Earth, lens, and source [32].

The amplification factor is determined by the density of the lensing mass, and is greater than 1.34 if the line of sight to the source star passes within the lens’s Einstein ring of radius

$$r_E^2 = \frac{4GM D_S}{c^2} x(1-x)$$

where D_S is the distance to the source and $x D_S$ is the distance to the lensing mass. The “optical depth”, a useful proxy for the mass of the lensing object, is given by the probability that at any given time the source star’s brightness is amplified by more than 1.34 [78]:

$$\tau = \frac{4GM D_S^2}{c^2} \int_0^1 \rho(x) x(1-x) dx \quad (1.2.1)$$

where ρ is the mass density of lenses.

Paczynski observed that while many had attempted microlensing with quasars over vast cosmological distances, observing stars in the halo of our own galaxy provides a much shorter and more convenient timescale of brightness fluctuations. Furthermore, while the optical depth for local halo stars is very small, their optical depth is enhanced if MACHOs compose a significant fraction of the dark halo mass [170].

Various surveys of the Large Magellanic Cloud have been performed (by collaborations such as MACHO, EROS, and OGLE) by scanning through many light curves and tagging sources with brightness variations characteristic of microlensing. By estimating detection efficiency and modeling the optical depth for a variety of MACHO scenarios, it is possible to constrain the MACHO composition of the galactic halo. While results of the MACHO collaboration give an upper contribution of $\sim 20\%$ [120], EROS-2 has pushed the limit down to 8% for a wide range of MACHO masses [78]. These results, at the very least, exclude MACHOs as the primary component of dark matter.

1.2.2 Modified Newtonian Dynamics

In 1982, Milgrom observed that if Newtonian forces are modified on a certain acceleration scale, a phenomenological model could explain anomalous galactic rotation curves (see Sec. 1.1.2). This hypothesis was called Modified Newtonian Dynamics (MOND).

In his original paper [162], Milgrom proposed a modification to Newton’s 2nd Law,

$$\vec{F}_g = m_g \vec{g} = m_g \mu\left(\frac{|\vec{a}|}{a_0}\right) \vec{a} \quad (1.2.2)$$

where m_g is the gravitational mass of an object with acceleration $\vec{a}$. The parameter a_0 is considered a new universal constant, an acceleration scale which has been obtained from a

sample of well-measured galaxies [219]:

$$a_0 = (1.20 \pm 0.27) \times 10^{-10} \frac{\text{m}}{\text{s}^2}$$

The function μ is chosen such that $\mu(x \gg 1) \approx 1$ and $\mu(x \ll 1) \approx x$, and is often of the form [84, 188]

$$\mu(x) = \frac{x}{\sqrt{1+x^2}} \quad (1.2.3)$$

which results in a force quadratic in a in the low acceleration limit. Using the centripetal force for mass m_g with orbital velocity v about a central mass M , such a law yields:

$$\begin{aligned} \frac{GMm_g}{r^2} &= \frac{m_g}{a_0} \left(\frac{v^2}{r} \right)^2 \\ \implies v^4 &= GMa_0 \end{aligned} \quad (1.2.4)$$

It is therefore a built-in feature of MOND that the velocity curve is asymptotically flat. For many galaxies, MOND accurately predicts rotation curves, essentially by tuning only the mass-to-light ratio. Example MOND galactic rotation curves are shown in Fig. 1.3.

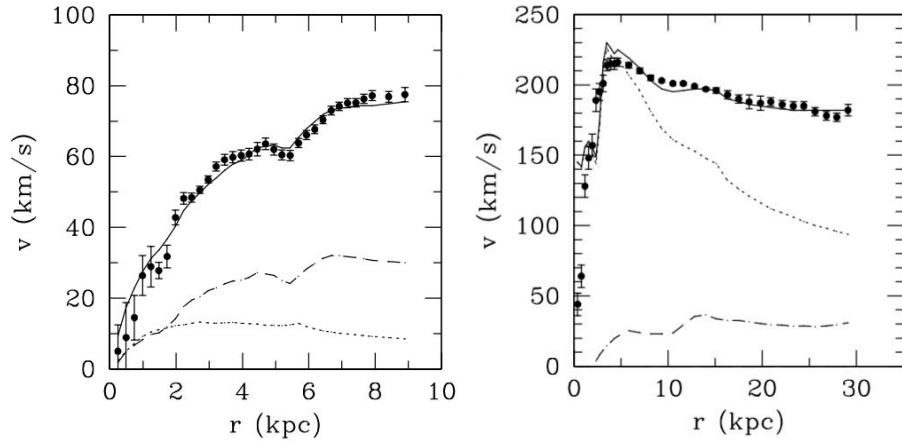


Figure 1.3: Rotation curves for two galaxies with very different surface brightness profiles, NGC 1560 and NGC 2903, with the solid lines representing the MOND fits [200].

Non-relativistic MOND is successful as a set of phenomenological rules, however is without a variational principle and actually violates conservation laws (specifically the conservation of linear momentum [200]). It took decades for such a relativistic, covariant theory to

emerge that reduces to MOND in the appropriate limit; the theory is called Tensor-Vector-Scalar Theory (TeVeS) since it incorporates the metric tensor $g^{\mu\nu}$, a dynamical vector field U^α , and a dynamical scalar field ϕ . The full theory is given by the action provided by Bekenstein [60, 213].

While the TeVeS theory successfully yields galactic dynamics and gravitational lensing, and reduces to general relativity, it requires the addition of fourth-generation “sterile” neutrinos with substantial mass to achieve even crude agreement with large-scale cosmological observations such as the CMB power spectrum (Fig. 1.4). Even the best fit TeVeS model requires a higher relic density of 15 eV sterile neutrinos ($\Omega_\nu h^2 \approx 0.156$) than the Λ CDM model predicts for dark matter ($\Omega_c h^2 \approx 0.12$) [241]. A “missing mass” component is therefore still required, and contriving explanations for this component of unidentified matter (e.g. sterile neutrinos, dark baryons) is contrary to the original motivation of MOND.

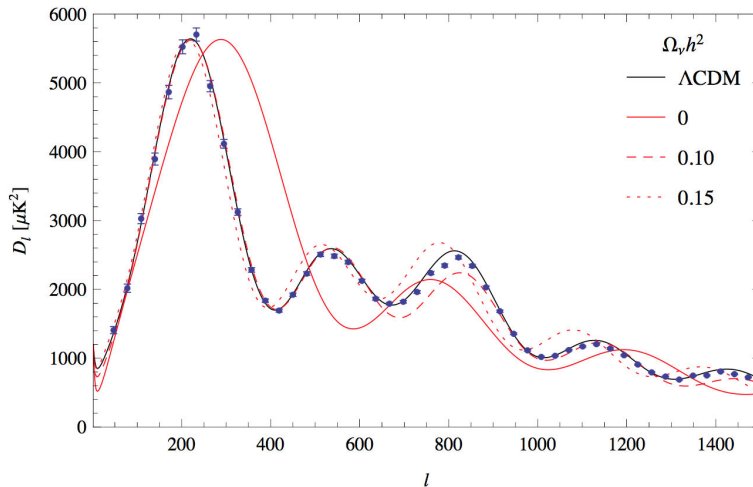


Figure 1.4: Planck data from 2013 fit with standard Λ CDM (black) and TeVeS with various sterile neutrino relic densities (red) [241].

1.2.3 Axions and Axion-Like-Particles (ALPs)

Another class of candidates for dark matter emerged from a theoretical solution to the “strong-CP problem” in particle physics. It was discovered that the complex vacua of QCD

naturally yield Lagrangian terms proportional to a phase parameter θ [172]. This gives a Lagrangian term of the form

$$\mathcal{L}_\theta = \theta \frac{g^2}{32\pi^2} F_a^{\mu\nu} F_{a\mu\nu} \quad (1.2.5)$$

CP-violation in strong interactions should therefore be evident unless θ is extremely small. There is no observed violation of the charge-parity (CP) symmetry in strong interactions; for example, strong bounds from the neutron electric dipole currently constrain $\theta < 10^{-9}$ [172]. This fine-tuning of the strong sector of the Standard Model is the strong-CP problem.

Perhaps the most well-motivated and promising solution is the introduction of a global chiral $U(1)_{PQ}$ Peccei-Quinn symmetry, which is spontaneously broken at some energy scale f_a and generates a Nambu-Goldstone boson known as the axion. This axion field effectively replaces the CP-violating angle θ and introduces new interactions.

Axions arising from symmetry breaking with f_a at the electroweak scale have been discounted [19, 41], however so-called “invisible axions” at much higher energy scales are still viable candidates for dark matter (as in the DFSZ and KSVZ models). In addition to QCD axions, particle excitations of orthogonal fields (called Axion-Like-Particles, or ALPs) are also sought after. Axions and ALPs may be observable in detectors through their coupling to photons, electrons, and nuclei.

There is a preferred mass range of $1 - 100 \mu\text{eV}$ for QCD axions, but the axion-photon coupling is expected to be extremely small over this mass range. The axion haloscope is a promising technique of achieving sensitivity in this channel. ADMX is such an experiment, which uses a cold microwave resonator immersed in a strong magnetic field to detect current oscillations over a range of frequencies. The principle of invisible axion exclusion at extremely small masses ($2.66 - 2.81 \mu\text{eV}$) has recently been shown [89].

An additional detection channel for both axions and ALPs is the axioelectric process, by which axions scatter off of electrons in a process analogous to the photoelectric effect. The axioelectric cross-section is given by [41]

$$\sigma_{Ae} = \sigma_{pe}(E_A) \frac{g_{Ae}^2}{\beta_A} \frac{3E_A^2}{16\pi\alpha_{em}m_e^2} \left(1 - \frac{\beta_A^{2/3}}{3}\right) \quad (1.2.6)$$

where σ_{pe} is the photoelectric cross-section for the medium, E_A is the axion energy, g_{Ae} is the axioelectric coupling, β_A is the axion velocity over the speed of light, α_{em} is the fine structure constant, and m_e is the electron mass.

Dark matter experiments using noble elements (e.g. xenon) as a detection medium are sensitive to axions or ALPs through this coupling; LUX, XENON100, and PandaX have already published exclusion limits over a combined mass range of $1 - 40$ keV/ c^2 , with a limit on g_{Ae} on the order of 10^{-13} [19, 41, 104].

A specific example of an ALP is the super-weakly interacting massive particle (super-WIMP), possibly resulting from the decay of a more massive, metastable relic WIMP. While fermionic super-WIMPs (e.g. gravitinos, sterile neutrinos) either are excluded as the primary dark matter component or are impossible to detect, bosonic super-WIMPs are an ALP that may be detectable through an axioelectric coupling with electrons [179]. Direct detection constraints have already been published for such couplings specifically [43].

The search for axions and ALPs is ongoing, with much phase space left to explore.

1.2.4 Hot Dark Matter and Neutrinos

In the 1970s, cosmologists realized that relic neutrinos would have a similar abundance to CMB photons, since there are conversion processes at thermal equilibrium in the early universe. Eventually the neutrinos froze out, but if they were massive ($m_\chi \sim 3$ eV), they could modify the large-scale structure. This marked the beginning of the shift away from baryonic matter as an explanation for the missing cosmological mass. Some early explorations of massive neutrinos can be found in [203] and [237].

“Hot dark matter” (HDM) describes such a class of particles, which decouple from other particles while they are relativistic. However, there are issues with this hypothesis [199]:

1. These particles are too energetic, washing out density fluctuations on shorter scales.
2. There are heavy constraints on the number density of neutrinos in a galactic halo, requiring neutrinos of significant mass.

It is known that “free-streaming” of particles smooths homogeneities, due to particles moving from over-dense to under-dense regions. Free-streaming is a form of collisionless damping which introduces a short wavelength cutoff in the perturbation spectrum, effectively washing out density fluctuations in the early universe on a shorter scale than the free-streaming distance (on the order of 700 light-years, or 200 parsecs) [199], and the first structures to form are supercluster size ($\sim 10^{15} M_\odot$) [136]. This would result in anomalous “top-down” structure formation, where superclusters form before smaller structures.

Secondly, fermionic constraints give an upper bound on the neutrino number density in galaxies, which then gives a lower bound for neutrino mass if they comprise most of the dark matter. For neutrinos to form a halo with a reasonable velocity spread of 100 km/s, 30 eV neutrinos are required [199]. For specifically dwarf spheroidal galaxies, the constraint is $m_\nu \sim 300 - 500$ eV, which is well outside cosmological bounds [136].

Simulations of hot dark matter models yield a universe with incorrect structure formation (the universe in such models does not form until a redshift of ~ 2) [199]. This constraint, along with constraints from galactic rotation curves, all but rule out HDM as a major component of dark matter. However, semi-relativistic dark matter of intermediate mass ($m_\chi \sim \mathcal{O}(\text{keV})$) serves as a more promising candidate. So-called “warm dark matter” (WDM) is appealing since it solves a number of small-scale issues with standard non-relativistic DM models (see Sec. 1.2.5) [74, 234]:

- The observed lack of theoretically predicted satellites of the Milky Way.
- Dark matter halos forming high-density (“cuspy”) centers compared to the observationally preferred constant density cores.
- Difficulties in producing typical disks due to mergers down to redshifts as low as $z \approx 1$.
- An excessive number of galaxies filling voids.

WDM potentially fixes these issues by suppressing structures of smaller size than its free-streaming length $\mathcal{O}(1 \text{ Mpc})$, since WDM particles have non-negligible velocities at high redshifts which delays the halo and star formation periods [152].

Various cosmological constraints and observations have somewhat disfavored WDM as a likely dark matter candidate. Recent studies have given a lower bound of $m_\chi \gtrsim 1 - 3$ keV for general WDM (i.e. decoupled thermal relics) and $m_\chi \gtrsim 5 - 10$ keV if the WDM is composed of sterile neutrinos [74, 152, 234]. There is remaining phase space for exploration, however, with WDM candidates such as axions or ALPs.

1.2.5 Cold Dark Matter and the Λ CDM Model

“Cold dark matter” (CDM) describes particles which decouple from other particles while they are non-relativistic. Such models naturally became popular, since they address the aforementioned problems with HDM [199]:

1. The Jeans length in CDM is zero, meaning there is no lower limit on the masses that can first gravitationally collapse. Fluctuations grow despite oscillations in the baryon-photon fluid (see Sec. 1.1.3), leading to the correct structure formation.
2. Since there is a very low velocity spread in CDM, there is no limit on the CDM density comprising the halo of low-mass galaxies.

The most popular and well-established cosmological model is Λ CDM, which incorporates dark energy (denoted by parameter Λ) in addition to CDM. To understand this model, we start with Einstein’s equation (Eq. 1.1.18) and examine the dynamics of cosmological fluids in an expanding universe.

Since Einstein’s equation can theoretically be satisfied for any choice of metric, let us make assumptions about spacetime and impose physical constraints on $T_{\mu\nu}$. Let us assume that spatial dimensions form a maximally symmetric 3-manifold, meaning that space is both homogeneous and isotropic (a generalization of translational and rotational invariance) [73]. This leads to the famous Friedmann-Lemaitre-Robertson-Walker (FLRW) metric, which is often used in standard cosmological models. This metric gives the interval

$$g_{\mu\nu} dx^\mu dx^\nu = ds^2 = dt^2 - a^2(t) \left[\frac{dr^2}{1 - \kappa r^2} + r^2 (d\theta^2 + \sin^2 \theta d\phi^2) \right] \quad (1.2.7)$$

where $a(t)$ is a dimensionless “scale factor” on all spatial dimensions and κ is a curvature parameter. For this choice of metric, one can solve for the Ricci tensor by calculating the Christoffel symbols which yield the Riemann tensor, then contracting with the metric. The Ricci scalar is ultimately given by [174]

$$R = -g \left[\frac{\ddot{a}}{a} + \left(\frac{\dot{a}}{a} \right)^2 + \frac{\kappa}{a^2} \right] \quad (1.2.8)$$

where the derivatives are taken with respect to t .

Let us study the case of a perfect cosmological fluid with isotropic rest frame pressure P and rest frame energy density ρ . Since the tensor is coordinate-independent, we may as well use the rest frame Einstein tensor:

$$T^{\mu\nu} = (\rho + P)U^\mu U^\nu - g^{\mu\nu}P = \text{diag}(\rho, -g^{ii}P)$$

Using Eq. 1.2.8 with Eq. 1.1.18 allows us to write out the temporal ($\mu = 0$) and spatial ($\mu = i$) parts as two separate equations, known as the general Friedmann equations [174]:

$$H^2(t) = \left(\frac{\dot{a}}{a} \right)^2 = \frac{8\pi G}{3}\rho - \frac{\kappa}{a^2} \quad (1.2.9)$$

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3P) \quad (1.2.10)$$

$H(t)$ is known as the Hubble parameter, as Hubble observed that the universe was in fact expanding at a rate governed by such a parameter (the Hubble parameter at the present epoch is the Hubble constant H_0).

We can now introduce a density parameter Ω , which is the sum of energy densities in the universe not due to curvature:

$$\Omega(t) = \sum_i \Omega_i(t) = \frac{8\pi G}{3H^2(t)} \sum_i \rho_i(t) = \sum_i \frac{\rho_i(t)}{\rho_{\text{crit}}(t)}, \quad \rho_{\text{crit}}(t) \equiv \frac{3H^2}{8\pi G} \quad (1.2.11)$$

ρ_{crit} is known as the critical density since departures from $\rho = \rho_{\text{crit}}$ would imply a non-zero spatial curvature. Since observations give $\Omega \approx 1$, we will hereafter assume $\kappa = 0$ [176].

We then relate the i th component of the energy density at time t to the present-day component, denoted by subscript 0:

$$\frac{\Omega_{i,0}}{\Omega_i} = \frac{\rho_{\text{crit}}}{\rho_i} \cdot \frac{\rho_{i,0}}{\rho_{\text{crit},0}} = \frac{H^2}{H_0^2} \left(\frac{a_0}{a} \right)^{n_i}$$

where n_i is a power which encodes how the i th density scales with $a(t)$. This allows us to rewrite Eq. 1.2.9 in terms of present-day energy density components:

$$H^2(t) = H_0^2 \left[\sum_i \Omega_{i,0} \left(\frac{a(t)}{a_0} \right)^{n_i} \right] \quad (1.2.12)$$

Furthermore, we can heuristically derive n_i for the various components of our universe. For the radiation (or relativistic) component, we observe that temperature scales as the inverse of the size of the system due to adiabatic expansion (a condition of thermal equilibrium) [190]. By the Stefan-Boltzmann law, the scaling of the radiation energy density is then

$$\rho_{\text{rad}} \propto T^4 \sim a^{-4}$$

For a non-relativistic matter component, assuming that the number density of particles is stable in thermal equilibrium, dilution through expansion gives $n(t) \propto a^{-3}$. Since the energy density scales with the mass density, we also get

$$\rho_M(t) \sim m \cdot n(t) \propto a^{-3}$$

Lastly, since the dark energy driving the expansion of the universe can be equivalently written as a cosmological constant term, we can assume a constant energy density that therefore scales as $a^0 = 1$. Combining all this, we get

$$H^2(t) = H_0^2 \left[\Omega_{\Lambda,0} + \Omega_{M,0} \left(\frac{a(t)}{a_0} \right)^3 + \Omega_{\text{rad},0} \left(\frac{a(t)}{a_0} \right)^4 \right] \quad (1.2.13)$$

Note that Ω_M includes both baryonic and dark matter, and that Ω_{rad} includes the neutrino component Ω_ν in the early universe, when neutrinos were highly relativistic.

Fits to precise cosmological data, such as the CMB power spectrum (Fig. 1.5), have heavily constrained these density parameters. The Planck experiment has precisely measured temperature deviations across angular regions of the CMB. The measured temperature anisotropies are used to create a power spectrum, in the form of a multipole expansion indexed by ℓ . This spectrum is information rich, since the relative strengths and phase of resonance peaks highly depends on the model parameters. The relative amplitudes of the

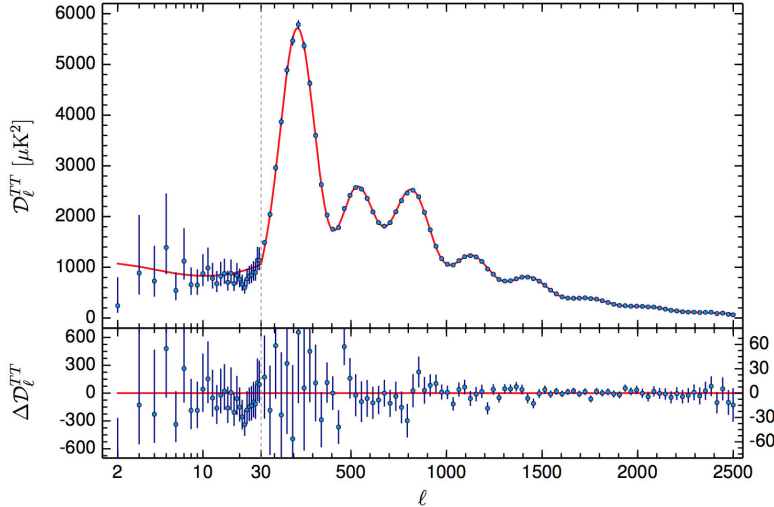


Figure 1.5: The 2015 Planck results for the primordial temperature power spectrum, fit exceptionally well with Λ CDM (red) [176].

first, second, and third peaks give information about the spatial curvature (Ω_κ), baryonic matter density (Ω_b), and DM density (Ω_{DM}). The precise relationship between the initial inflationary perturbations, the various cosmological model parameters, and the temperature anisotropies is beyond the scope of this thesis, but for discussions see [136, 229, 231].

Using parameters which are consistent with other cosmological data (recently found to be $\Omega_b = 0.048$, $\Omega_{DM} = 0.26$, $\Omega_\Lambda = 0.692$, $\Omega_{\text{rad}} \sim 10^{-5}$, $\Omega_\nu < 0.0014$) [225], the Λ CDM model fits the data extremely well. Λ CDM is perhaps the most promising model for matching cosmological observations, both because of its simplicity and because of its ability to simultaneously reproduce many different phenomena.

1.3 The WIMP Hypothesis: A Promising Avenue

1.3.1 The WIMP Miracle

If dark matter is indeed cold, then the WIMP (Weakly Interacting Massive Particle) is a promising candidate. One of the original motivations for pursuing weakly interacting DM came from early universe cosmology.

Let's presume that in the hot, dense early universe, a dark matter particle of mass m_χ existed in a sea at a temperature $T \gg m_\chi$ at thermal equilibrium with Standard Model (SM) particles [125]. If creation and annihilation processes for this particle were equally efficient, how does such a particle survive complete self-annihilation? There are many proposals [214]:

1. An unknown physical mechanism for particle-antiparticle asymmetry, which fixes the final DM abundance given a sufficiently large annihilation cross section.
2. The DM does not interact with the SM particles, and its abundance was set by initial conditions. (This is the case with the axion “misalignment mechanism”, by which the QCD vacuum parameter θ is shifted from the axion field's minimum potential, resulting in coherent oscillations that fix the initial energy density of the DM [91].)
3. SM particles are produced at early times in a “dark sector” extension of the SM, which then decay to DM, resulting in net DM production at later times.
4. The DM abundance is initially negligible, and interacts with the bath of SM particles so feebly that when $T < m_\chi$ there is net DM production (this is called “freeze-in”) [112].
5. Hubble dilution competes with self-annihilation of the particle, leading to “freeze-out” of the DM number density as these particles veer away from thermal equilibrium.

The last “thermal relic” scenario is perhaps the most enticing, since the late-time relic abundance can be entirely determined by the cross section for the annihilation process for a broad class of models. Furthermore, the remaining DM abundance in such a model is independent of the uncertain early thermal history of the universe and possible new interactions at high scales [112].

This scenario unfolds as follows. As the universe expands and cools to temperatures below the particle mass ($T < m_\chi$), creation processes become suppressed. On the other hand, annihilation processes continue as the particle finds its antiparticle. At thermal equilibrium,

the particle number density then falls off according to the Boltzmann distribution

$$n_\chi = g_\chi \left(\frac{m_\chi T}{2\pi} \right)^{3/2} e^{-m_\chi/T} \quad (1.3.1)$$

where g_χ is the number of internal degrees of freedom for particle χ . The competing effects of expansion and annihilation are described by the Boltzmann equation [125]:

$$\frac{dn_\chi}{dt} + 3Hn_\chi = -\langle \sigma_{\chi\bar{\chi}} v \rangle (n_\chi^2 - n_{\chi,\text{eq}}^2) \quad (1.3.2)$$

where the term containing the Hubble parameter H governs dilution and $\langle \sigma_{\chi\bar{\chi}} v \rangle$ is the thermally-averaged self-annihilation cross-section of the particle. This cross-section determines the freeze-out temperature at which the “comoving” number density, or the particle density expansion-normalized by a factor of $1/a^3$, becomes constant (see Fig. 1.6).

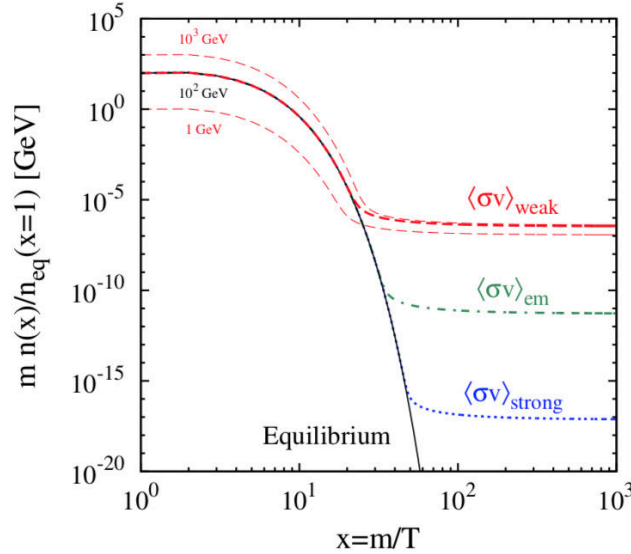


Figure 1.6: The solid curve is the particle number density in thermal equilibrium, while the dashed curves represent the densities based on various self-annihilation cross-sections (with multiple masses shown for the weak scale). $x = m/T$ serves as a proxy for time. [221]

While solving this equation can be done numerically, we can do a crude estimate of the cross-section which gives a relic density consistent with cosmological observations. From Eq. 1.3.2, we can see that in the limit that $T \ll m_\chi$,

$$\langle \sigma_{\chi\bar{\chi}} v \rangle \sim \frac{H_f}{n_f} \quad (1.3.3)$$

where n_f is the number density which becomes constant at “freeze-out”, or when the expansion rate becomes comparable to the rate of annihilation.

In a radiation-dominated early universe, the sum of energy densities is approximately given by just the radiation component, giving the freeze-out Hubble parameter:

$$H_f^2 \sim \frac{8\pi G}{3} \rho_{\text{rad}}, \quad \rho_{\text{rad}} = \frac{4\sigma_B T_f^4}{c^3} \quad (1.3.4)$$

We can relate n_f to the particle’s mass m_χ and relative energy density Ω_χ using

$$\Omega_\chi = \frac{8\pi G}{3H_f^2} \rho_f = \frac{8\pi G}{3H_f^2} n_f m_\chi = \frac{8\pi G}{3H_0^2} \left(\frac{a_f}{a_0}\right)^3 n_f m_\chi \quad (1.3.5)$$

Given that $T \sim 1/a$ (see Sec. 1.2.5), we can relate the temperature at freeze-out to the observed temperature of the CMB:

$$\frac{T_{\text{CMB}}}{T_f} \sim \frac{a_f}{a_0} \quad (1.3.6)$$

Combining Eq. 1.3.5 with Eq. 1.3.6,

$$n_f \sim \frac{3H_0^2 \Omega_\chi}{8\pi G m_\chi} \left(\frac{T_f}{T_{\text{CMB}}}\right)^3 \quad (1.3.7)$$

We can implement a further constraint for a given particle of mass m_χ and density Ω_χ ; we can solve for the ratio m_χ/T_f by relating Eq. 1.3.7 with the Boltzmann distribution from 1.3.1. This ultimately reduces to an equation of the form

$$\left(\frac{m_\chi}{T_f}\right)^{3/2} e^{-m_\chi/T_f} \propto \frac{\Omega_\chi}{m_\chi} \quad (1.3.8)$$

Since we have precise measurements of the relative dark matter density Ω_χ , we can choose m_χ and find the mass-to-temperature ratio. For a 100 GeV particle, this yields a relatively stable value of $m_\chi/T_f \sim 20$. Combining Eq. 1.3.3, 1.3.4, and 1.3.7 then gives a self-annihilation cross-section

$$\langle \sigma_{\chi\bar{\chi}} v \rangle \sim 10^{-26} \text{ cm}^3/\text{s} \quad (1.3.9)$$

Let us estimate a simple tree-level self-annihilation cross-section for such a particle. If we assume that the interaction vertex has a coupling constant on the scale of a standard weak interaction, i.e. $\alpha_\chi \sim g^2/4\pi \sim \mathcal{O}(0.01)$ [214], we get an annihilation cross-section of

$$\langle \sigma_{\chi\bar{\chi}} v \rangle \sim \frac{\alpha_\chi^2}{m_\chi^2} \sim 10^{-26} \text{ cm}^3/\text{s} \quad (1.3.10)$$

This so-called “WIMP miracle” is one reason why the WIMP became a popular candidate for dark matter. Cosmological constraints from the relic density of CDM particles naturally give an annihilation cross-section within an order of magnitude of a characteristic weak interaction for a broad range of particle masses ($m_\chi \sim 1 \text{ GeV} - 1 \text{ TeV}$). For a more precise treatment of freeze-out and relic densities, see [125, 136, 214, 221].

It is imperative to note that this “miracle” is a statement about cross-sections and does not necessitate weak interactions [45]. Given that both direct detection experiments have heavily constrained the WIMP phase space and indirect detection experiments have already begun to encroach on the “miraculous” self-annihilation cross-section (see Sec. 2.1.2), it is quite possible that the WIMP miracle is merely a coincidence and the dark matter is produced by alternate mechanisms.

1.3.2 Candidates for the WIMP

WIMPs are promising dark matter candidates for many reasons. They form a CDM in the universe which results in correct structure formation and reproduces a broad range of phenomena, including galactic rotation curves and gravitational lensing.

There is enormous discovery potential for WIMPs that couple to SM particles. Motivations already exist in particle physics for extensions to the SM, particularly at the weak energy scale. There are numerous extensions which predict viable WIMP candidates [189]:

- **Two Higgs Doublet Models (2HDM)** – An extra Higgs doublet is added to the SM. Fields may be added which couple to the new Higgs states and serve as WIMPs; alternatively, as in the inert doublet model (IDM), the lightest of the additional neutral Higgs bosons may interact as a WIMP via Higgs mediation with SM particles.
- **Little Higgs Models** – A light composite Higgs is used, with new heavy states introduced as partners of the top quark and/or as gauge bosons. This model may produce a WIMP as either a scalar particle or a heavy photon-like vector boson.
- **Twin Higgs** – There is a twin sector mirroring the SM, the lightest Higgs of the

combined sector serving as the pseudo-Goldstone boson. A member of this twin sector may be a WIMP that couples with SM particles via Higgs mediation, as with IDM.

- **Kaluza-Klein States** – In models with compactified universal extra dimensions (UED), SM particles can propagate in a new dimension, producing Kaluza-Klein (KK) states by appearing as heavier copies of SM particles. WIMPs may arise as the lightest KK state, often a heavy version of the hypercharge gauge boson. Minimal UED theories have been largely ruled out at the Large Hadron Collider (LHC).
- **Supersymmetric Particles** – Supersymmetry (SUSY) models are extensions of the SM which include additional “superpartners” based on a set of supersymmetry transformations. The lightest stable partner generated in such a model may have WIMP-like properties. SUSY, a very popular theory for generating WIMPs, covers an enormous range of detectable phase space and is discussed in the next section.

1.3.3 Supersymmetric Models

In the current SM, we do not have a Lagrangian for particle physics at all scales, but rather effective Lagrangians that operate below a certain energy cutoff scale (so-called “effective field theories”, or EFTs).

Scalar fields of these EFTs have VEVs (vacuum expectation values) which spontaneously break gauge symmetries, such as the electroweak symmetry. These Nambu-Goldstone bosons, like the Higgs particle, acquire mass of order Λ (the scale of the cutoff energy) because of radiative corrections like virtual loops, which come in the form [131]

$$\delta m_{\text{scalar}}^2 \sim g^2 \Lambda^2 \tag{1.3.11}$$

Since we do not observe the effects of such a mass, we have to fine-tune couplings by 10^{28} ; this is called the “naturalness problem”. One way to avoid this problem is with SUSY.

The theory places particles in multiplets, related by SUSY transformations which send particles to their partners with spin either raised or lowered by $1/2$. This introduces bosonic

loop diagrams wherever fermionic loops exist and vice versa, cancelling divergences that normally have to be corrected away. This could solve the naturalness problem, however superpartners have not yet been discovered at collider experiments, so we know that supersymmetry must be broken at some higher energy scale. The mass splittings in supermultiplets should not be much greater than the electroweak scale ($\mathcal{O}(1 \text{ TeV})$) in order for it to be an answer to the fine-tuning problem [131].

A popular subset of SUSY models is the MSSM space; these theories include all of the original SM fields, with additional SUSY partners and an extra Higgs doublet. The most important ingredient for determining allowed interactions is “ R -parity”, given by

$$R = (-1)^{3(B-L)-2S} \quad (1.3.12)$$

where B is baryon number, L is lepton number and S is the spin. $R = 1$ for ordinary particles and -1 for superpartners. If R -parity were broken, there would be no selection rules to prevent the decay of SUSY particles of light mass ($m \gtrsim 1 \text{ GeV}$), leaving no viable candidates for dark matter. In addition, there would have to be heavy constraints in order to not violate baryon and lepton number. If R -parity is conserved, however, the lightest R -odd particle is absolutely stable, and is called the Lightest SUSY Particle (LSP).

The most likely LSP is the “neutralino” (a SUSY counterpart of the neutrino). The neutralino is a combination of the “bino” $\tilde{B}$ (superpartner of the $U(1)$ gauge field B), the “wino” $\tilde{W}$ (superpartner of the $SU(2)$ gauge field W), and the “higgsino” $\tilde{H}$ (superpartner of the neutral Higgs bosons):

$$\chi = N_{10}^* \tilde{B} + N_{20}^* \tilde{W}^3 + N_{30}^* \tilde{H}_1^0 + N_{40}^* \tilde{H}_2^0 \quad (1.3.13)$$

The neutralino is the likeliest LSP for the following reasons [131]:

- Charginos or sleptons would have relic densities such that they show up in anomalously heavy proton searches, and they don’t.
- Squarks or gluinos would be expected to form hadrons, which we don’t observe; regardless, they are unfavorable in theory due to their being more massive than other particles (sleptons and neutralinos respectively).

- Sneutrinos either have larger mass than sleptons or are largely ruled out by WIMP direct-detection experiments.
- Neutralinos are stable and weakly-interacting, with remaining phase space to explore.

This SUSY model therefore provides an enticing WIMP candidate: its likely LSP, the neutralino. However, there is an enormous landscape of SUSY theories, making it difficult to compare theory with observation. The “unconstrained MSSM” (uMSSM) comes with 105 parameters (excluding the SM), making the model useless in any predictive or phenomenological capacity, however various levels of constraint may be applied [64].

This may be reduced to the “phenomenological MSSM” (pMSSM), which only has 19 unknown parameters, if we make the following assumptions:

1. No new source of CP violation.
2. No flavor changing neutral currents.
3. SUSY breaking scalar masses are the same for the first and second squark generations.

While the enforcement of these constraints is well-motivated by experimental data, the pMSSM still has an enormous phase space which is difficult to exclude. Various assumptions can be made which further reduce the number of free parameters, leading to variations of the pMSSM (i.e. pMSSM n has n parameters) [235].

There is also the popular “constrained MSSM” (cMSSM) theory, which comes from the additional major assumption of parameter unification at some grand unified theory (GUT) scale. There are only 5 free parameters: the common scalar and gaugino masses m_0 and $m_{1/2}$, the common trilinear coupling A_0 , the ratio of the two Higgs VEV values $\tan \beta$, and the Higgs mass parameter μ [56]. This is made possible by extrapolating the low-energy SUSY-breaking parameters up to some high energy scale where they unify, requiring electroweak symmetry breaking conditions to produce the observed couplings [235].

This is an explorable solution to the naturalness problem which is well-motivated by minimal supergravity (mSUGRA) models, in which SUSY-breaking occurs in a hidden sec-

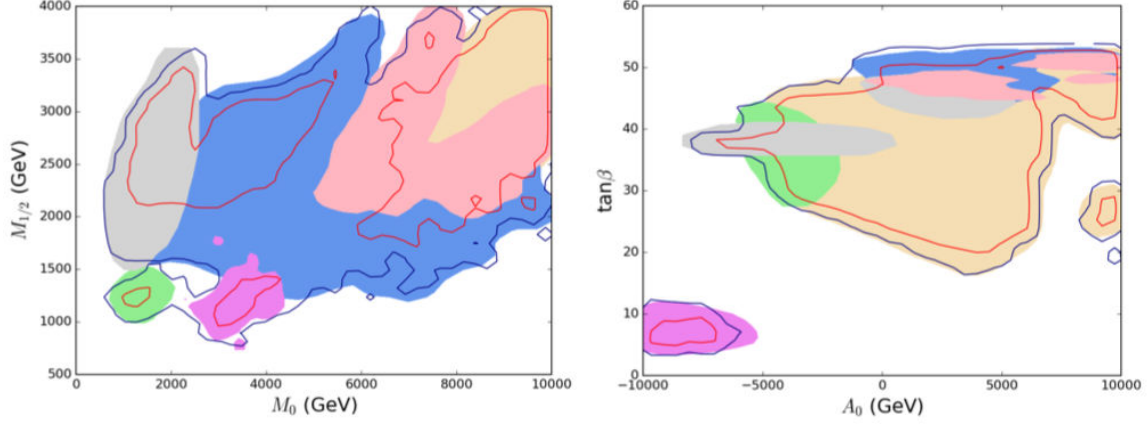


Figure 1.7: Allowed parameter space of the cMSSM after implementing constraints from precision electroweak and B -physics measurements, LHC Run 1 and Run 2 SUSY searches, observed DM relic density, and LUX Run 3 and Run 4 direct detection limits. Color regions indicate different LHC production channels, red and blue contours are the 68% and 95% CL regions obtained from likelihood analysis. [116]

tor which communicates with the visible sector only through gravitational interactions [64]. While these two models are often quoted interchangeably, they are separate theories and mSUGRA imposes additional constraints which further reduces the number of free parameters [90]. As a result, phenomenological constraints on the cMSSM (unlike true mSUGRA models) are shown on a $(m_{1/2}, m_0)$ plane for fixed A_0 , $\tan\beta$, and $\text{sgn}(\mu)$ (see Fig. 1.7).

Chapter 2

Detecting WIMPs

If we are to discover WIMPs, it is crucial that searches be done from a variety of experimental angles. There is no superior, clear-cut method for DM detection, since they all have their experimental advantages and drawbacks. Furthermore, the various methods of detection complement and inform each other by exploring different corners of parameter space and influencing the next generation of experiments.

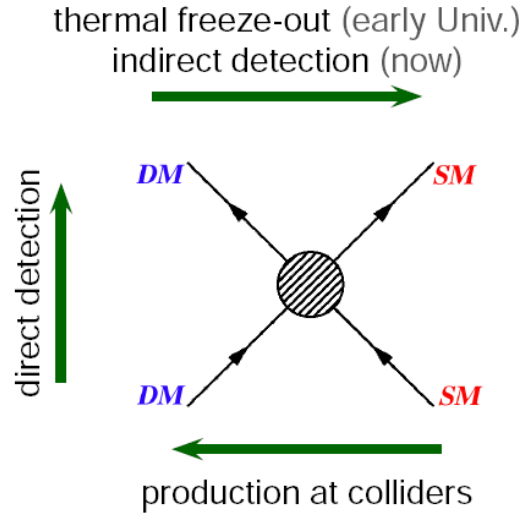


Figure 2.1: A generic Feynman diagram of DM-SM interactions, with green arrows indicating the direction of time and the mode of detection.

Fig. 2.1 illustrates the different modes of DM detection. In this chapter we will give an

overview of the techniques and latest results for production, indirect detection, and direct detection of DM.

2.1 Modes of Detection

2.1.1 Direct Production

Dark matter particles, or more precisely particles from the “dark sector” (including mediators of beyond-SM interactions), may be directly produced at high-energy experiments such as the Large Hadron Collider (LHC). At the LHC, pp collisions produce many annihilation products, and events are reconstructed by detecting and accounting for these products.

As mentioned previously, there are effective field theories (EFTs) which approximate interactions at some low-energy scale. Sometimes this is done by replacing the unknown mediation mechanism by a simple contact interaction, which may be useful for direct and indirect detection where model-independence is desired. However, since the LHC has high enough energy to probe dark sector mediators, “simplified DM models” for direct production include both DM and its mediators, bringing along the associated couplings and masses as parameters [71].

The CMS, ATLAS, and LHCb collaborations at the LHC are searching in many channels for dark sector particles. An overview of some of the effective Lagrangian operators which govern potential DM-SM interactions at the LHC is given by Tripathi et al. [46], but here is a brief summary of observable DM signatures as presented recently [71]:

- $E_T^{\text{miss}} + X_{\text{SM}}$: DM particles produced at the LHC escape without detection, resulting in missing transverse momentum energy E_T^{miss} . These events may come with a SM particle X (a “Mono- X ” signature) which tags the event. X may be a jet (hadronized quark or gluon), a photon, a vector boson (W or Z), a heavy flavor quark, or a Higgs.
- $E_T^{\text{miss}} + h$: In the specific case of a Higgs interaction, there is usually a mediator Z' which either radiates a Higgs then decays directly into DM (the “baryonic Z' ”), or

decays into a Higgs and an intermediate heavy particle which produces the DM (the “ Z' -HDM” model) [212]. See Fig. 2.2 for the latest limits on these models.

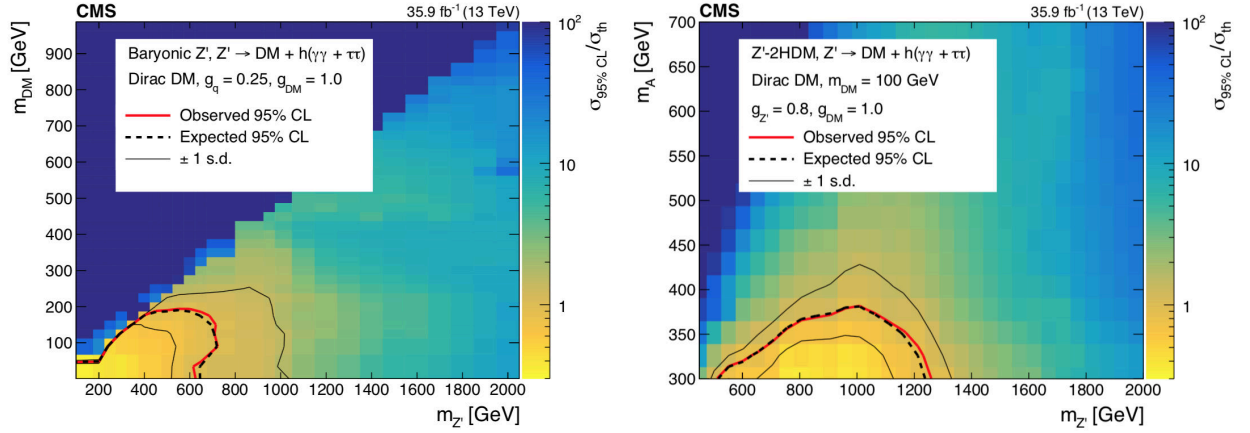


Figure 2.2: Recent exclusion limits set by CMS with 13 TeV pp collisions for the baryonic Z' (left) and Z' -HDM models (right), from [212]. Shown on the mediator-DM mass plane, with color scale indicating confidence in exclusion of theory.

- $E_T^{\text{miss}} + (t\bar{t}, b\bar{b})$: In this variation on the Mono- X signature, a scalar or pseudoscalar mediator (ϕ or a) couples strongly to heavy quarks, resulting in this mediator decaying into DM with final states including $t\bar{t}$ or $b\bar{b}$.
- Mono- Z' : In another variation on the Mono- X signature, a beyond-SM particle Z' decays hadronically into two jets. There are multiple models for this: (1) the Z' couples to dark-sector fermions χ_1 and χ_2 (one of which is the DM), (2) the Z' radiates a “dark Higgs” h_D , which then decays into DM.
- Mediator to (jj, ll) : Since the DM mediator would interact with SM particles, it may decay into dijet and dilepton final states.
- Dark Photon $A' \rightarrow \mu^+\mu^-$: Though this is a non-WIMP sector, it is worth noting an LHC search for alternative DM. If there exists a rich “dark sector” of new particles, mediators may couple to the SM via a dark “portal”. One proposed mediator is the massive “dark photon” A' , which couples to the SM and may decay into $\mu^+\mu^-$.

There are far too many results from the LHC to be presented here, but a collective summary of recent results is shown in [71]. Experiments at colliders have great sensitivity through proposed DM production mechanisms, however no evidence for DM has yet been found. It should be noted that there is still much phase space yet to explore, and only a small fraction of the collected LHC data has been analyzed.

2.1.2 Indirect Detection (Annihilation)

Indirect detection can be achieved by measuring the SM products resulting from annihilation or decay of dark matter particles. Such processes occurred in the early universe until thermal freeze-out (See Sec. 1.3.1), and are studied by astrophysicists in a variety of channels.

In general, the annihilation or decay products fall into two categories: neutral particles (photons and neutrinos) and charged particles (cosmic rays). These channels are treated very differently, since neutral particles travel to us in straight lines, whereas charged particles diffuse through local magnetic fields and have heavily altered energy spectra [214].

For neutral particles emitted from a solid angle $d\Omega$ subtended by a source at radius $\vec{r}$ with dark matter density ρ and an initial annihilation energy spectrum $(dN/dE)_0$, the signal spectrum received at our detector of area A per unit time is given by

$$\frac{dN}{dE dt} = \frac{A}{4\pi} \left(\frac{dN}{dE} \right)_0 \frac{\langle \sigma v \rangle}{2m_\chi^2} \int dr d\Omega \rho^2(\vec{r}) = \frac{A}{4\pi} \left(\frac{dN}{dE} \right)_0 \frac{\langle \sigma v \rangle}{2m_\chi^2} J_{\text{ann}} \quad (2.1.1)$$

We have introduced a useful “ J factor” here, which isolates the density profile of the DM (the astrophysics) from the particle physics.

For neutral particles that result from DM decays rather than annihilations, with a DM decay lifetime τ , the spectrum is given by

$$\frac{dN}{dE dt} = \frac{A}{4\pi} \left(\frac{dN}{dE} \right)_0 \frac{1}{2m_\chi \tau} \int dr d\Omega \rho(\vec{r}) = \frac{A}{4\pi} \left(\frac{dN}{dE} \right)_0 \frac{1}{2m_\chi \tau} J_{\text{dec}} \quad (2.1.2)$$

Decays integrate one less power of the mass density compared to annihilations, since only one power of the number density is required for such a process.

The J factors introduced here encode the dark matter distribution in a given region; with the particle physics fixed, this factor determines the observed signal spectrum. For example,

the galactic center of the Milky Way has $J_{\text{ann}} \approx 10^{22} \text{ GeV}^2/\text{cm}^5$, whereas dwarf satellite galaxies have $J_{\text{ann}} \approx 10^{17-20} \text{ GeV}^2/\text{cm}^5$. However, dwarf galaxies have less astrophysical backgrounds, so actually serve as cleaner targets for study [214].

Note that for more distant objects, where distortion of the spectra due to redshift z becomes significant, we have to integrate over the redshift dependence of the emission spectrum and density profile, as well as account for Hubble expansion. Furthermore, if we want to include absorption effects, we can include an additional factor of $e^{-\tau(E,z)}$ in the integral which parametrizes the optical depth of photons through the medium.

There are several categories of neutral particle spectra: hadronic continua (by which pions are produced, decaying into a broad spectrum of photons and charged particles), leptonic spectra (by which photons are only produced in 3-body final states), and spectral lines (by which monoenergetic $\gamma\gamma$ or $\nu\bar{\nu}$ pairs are produced by more rare processes). However, if DM circumvents SM processes by annihilating into “dark sector” particles, the range of possible spectra is expanded.

Some indirect searches probe cosmic ray signals, which introduces a new set of complications. Cosmic ray propagation is non-trivial, and the energy spectra evolve with distance due to interfering ambient magnetic fields. Thus, it is necessary to study diffusion equations to obtain a solution for the number density of annihilation products.

If we take $\psi(\vec{x}, E, t) \equiv dn/dE$, with n the number density for cosmic ray particles, the diffusion equation might take the general form [214]

$$\begin{aligned} \frac{\partial \psi}{\partial t} = & D(E) \nabla^2 \psi + \frac{\partial}{\partial E} (b(E) \psi) + \frac{\partial}{\partial z} (v_c \psi) \\ & - \frac{\psi}{\tau} + \frac{\partial}{\partial p} \left[p^2 D_{pp} \frac{\partial}{\partial p} \left(\frac{\psi}{p^2} \right) \right] + Q(\vec{x}, E, t) \end{aligned} \quad (2.1.3)$$

$D(E)$ is a diffusion coefficient, $b(E)$ is an energy loss term, v_c is the convection speed of particles out of the galactic plane, the $1/\tau$ term governs decay or fragmentation of unstable cosmic rays, the term with momentum p governs diffusive reacceleration, and Q is a source term. This equation may yield a power law for the expected signal which is sometimes possible to distinguish from background astrophysics.

There are many kinds of experiments to probe the many indirect search channels: X-ray and γ -ray telescopes (e.g. Fermi-LAT, Chandra, XMM-Newton, HESS, VERITAS), radio and microwave telescopes (e.g. Planck, WMAP), neutrino experiments (Super-K, IceCube), and cosmic ray experiments (e.g. AMS-02, AUGER).

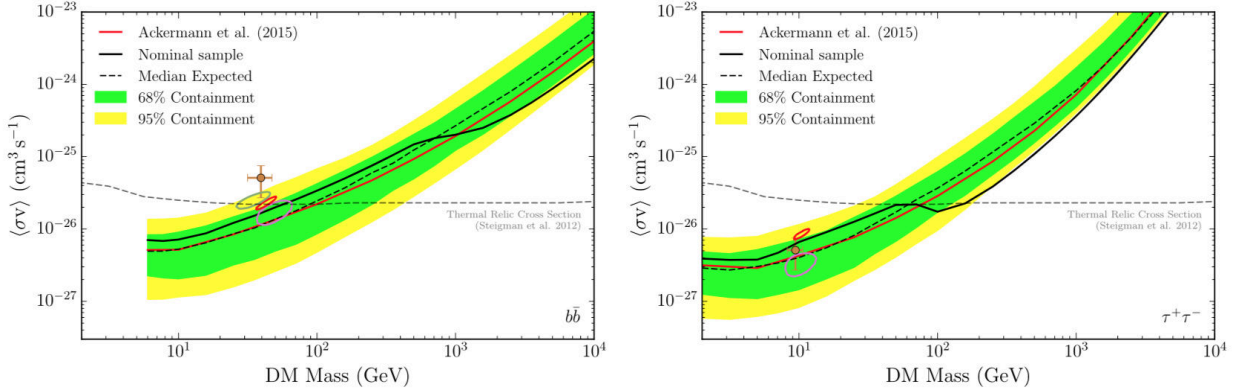


Figure 2.3: Upper limits (with 95% confidence bands) on the DM annihilation cross section for the $b\bar{b}$ and $\tau^+\tau^-$ channels, as presented by Fermi-LAT [228]. The dashed line shows the thermal relic cross-section constrained by observed DM abundance, and the closed contours represent DM claims from the GCE.

Potential DM signals have in fact been reported, though they are somewhat in tension with the most recent exclusion limits (see Fig. 2.3) [228]. There are multiple γ -ray excesses: a 3.5 keV line reported by XMM-Newton (which other experiments have confirmed [72], faintly detected [195], and strongly excluded [37, 130]), and the well-known Galactic Center Excess (GCE) which is seen as a broad peak in the energy spectrum at 1-3 GeV [8]. While the former is consistent with a decaying 7 keV sterile neutrino, the best fit results for the GCE indicate thermal relic DM of ~ 50 GeV annihilating to $b\bar{b}$.

There is also the cosmic ray positron excess which was detected by PAMELA and subsequently confirmed by both Fermi [4] and AMS-02, though there remains some uncertainty about its origin. The DM interpretation involves a very heavy particle with an annihilation cross-section well above the thermal relic value. Furthermore, there are various proposed mechanisms of positron production and propagation which may be responsible [214].

While indirect detection experiments have yielded more signals for DM interpretation than direct production searches at colliders, exclusion limits being set by other indirect searches are very close to ruling out these discoveries.

2.1.3 Direct Detection (Scattering)

Direct detection includes the elastic and inelastic scattering of DM particles with standard SM particles, resulting in measurable energy signatures. There are a vast number of detector types in this sector: single- and dual-phase noble element time projection chambers, solid state superconducting sensors, cryogenic calorimeters, and so on. General principles of direct detection and an overview of detector types will be discussed in Sec. 2.2.

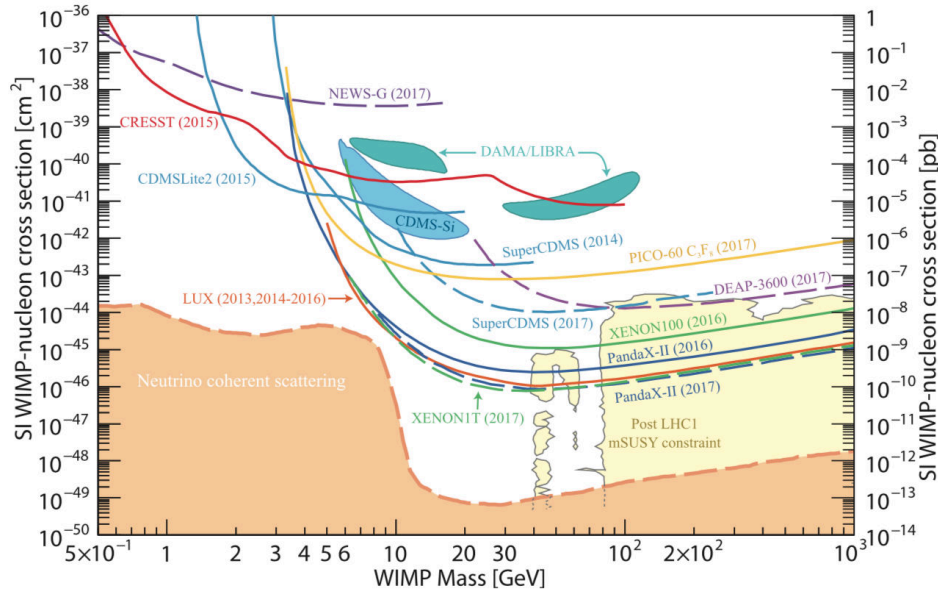


Figure 2.4: A summary of spin-independent WIMP interaction cross-section limits across a broad range of masses [225]. Colored contours represent claims by CDMS and DAMA/LIBRA, which have been excluded by numerous experiments.

In the absence of a DM signal, direct detection experiments quote dark matter search results as an exclusion limit curve on the DM-SM scattering cross-section; DM over a certain mass range is excluded based on null results (i.e. no statistically significant population of dark matter events was observed).

For WIMPs, which hypothetically undergo weak interactions with ordinary atomic nucleons, there are two types of limits which are published: spin-independent (SI) and spin-dependent (SD) interactions. The world's leading exclusion limits (as of 2017) for SI WIMP-nucleon scattering cross-sections is shown in Fig. 2.4, along with the DM discovery claims by CDMS and DAMA/LIBRA. Not only do existing limits exclude these discovery claims, but they also have begun to exclude the space of preferred SUSY models.

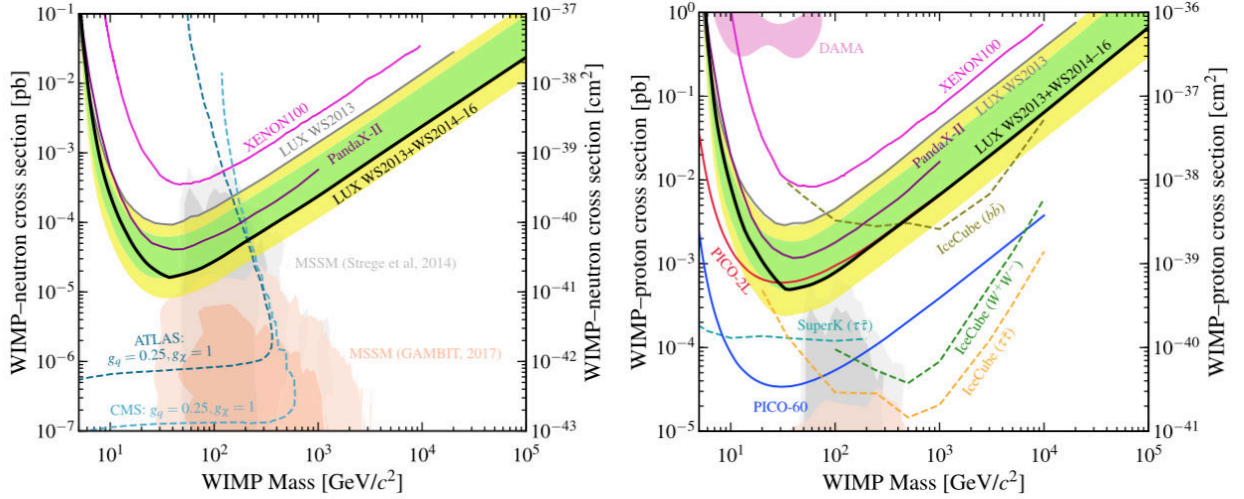


Figure 2.5: (Left) SD WIMP-neutron cross-section limits for direct detection experiments, with dashed lines indicating limits set by direct production at the LHC. (Right) SD WIMP-proton cross-section limits with dashed lines indicating limits by indirect searches. [20]

For the case of SD interactions, which distinguish between protons and neutrons, SD limits are presented separately for each nucleon type. In Fig. 2.5, WIMP-neutron and WIMP-proton SD limits for various experiments are shown, along with contours showing MSSM models and the excluded DAMA claim.

A number of claims for DM discovery have been made in the last decade, particularly modulation signals from DAMA/LIBRA [61], excess ionization signals in the germanium of CoGeNT [1], scintillation/heat signatures detected in CRESST-II crystals [38], and a few events in the silicon detectors of CDMS-II [5]. New datasets and/or reanalyses have resulted in the withdrawal of almost all claims [6, 86, 201], with the exception of DAMA/LIBRA. Furthermore, the many published exclusion limits and noted internal consistency issues of

the DAMA/LIBRA results [225] all but nullify previous claims for DM detection.

2.2 Principles of Direct Detection

2.2.1 Energy Deposition Channels in Matter

The direct detection of WIMPs is premised on interactions with ordinary atomic matter. WIMPs may interact with either the nuclei or atomic electrons of materials, imparting energy which produces an observable signature.

There are multiple channels for energy deposition: scintillation (photons produced through de-excitations of atomic electrons), ionization (charge produced by ionization of atoms along the particle track), and heat (phonons produced due to the motion of recoiling atoms). More exotic forms of detection do exist, e.g. bubble nucleation in superheated liquids [35, 36, 57, 58].

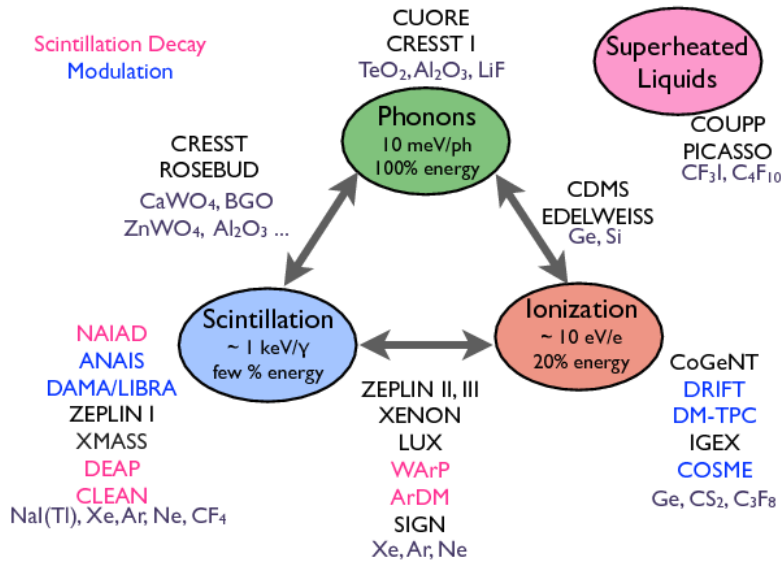


Figure 2.6: Energy deposition channels for various direct detection experiments [196].

Direct detection channels, and some past experiments corresponding to each, are shown in Fig. 2.6. There are technological challenges associated with each channel, however it is ideal to simultaneously measure multiple channels in order to have more handles for energy

reconstruction and particle identification. For example, scintillation-only detectors may use a detection medium such as inorganic NaI crystals, however materials with special micro-physical properties (e.g. noble elements) may yield both scintillation light and ionization electrons in a way that can be leveraged in dark matter searches.

The type of quanta being collected drastically changes the detection medium and requisite technologies. In the case of phonon detection, thermodynamic conditions must be tuned far more precisely than scintillation/ionization detectors, whereas for the latter light and charge collection must be optimized through characterization of optical and electrostatic properties of detector materials. Such challenges make combining more than two of these channels unfeasible, at least with current technologies.

2.2.2 Effective Field Theories and Scattering Cross Sections

In order to build a detector with good DM sensitivity, we have to maximize the probability of a WIMP interaction over a range of energies. The differential scattering cross section gives the probability of a WIMP-nucleus scatter, but is highly model dependent and its calculation requires assumptions. We will follow the treatment of [33] and [150] for this discussion.

As previously mentioned, effective field theories (EFTs) are used to maintain some model independence and compare experimental results with theory. Simple “effective Lagrangians” can be used to calculate cross sections in some low-energy limit. We start with a general Lagrangian which describes a fermionic WIMP interacting with a quark via mediator ϕ :

$$\mathcal{L}_{\text{eff}} = g(q^2, m_\phi) \bar{\chi} \Gamma_\chi \chi \bar{Q} \Gamma_Q Q \quad (2.2.1)$$

Here, the effective coupling g depends on mediator mass m_ϕ and momentum transfer q , Q is the quark field, and each Γ encodes the transformation properties of the field.

Let us first take the case of a simple contact interaction with no nuclear spin dependence, where $q^2 \ll m_\phi^2$ and $g \sim 1/m_\phi^2$. In this case, the canonical effective Lagrangian is

$$\mathcal{L}_{\text{eff}} = g \bar{\chi} \chi \bar{Q} Q$$

By calculating the contribution of each quark flavor to the nucleon fields (n and p), isolating the effective neutron and proton couplings (f_n and f_p), and rewriting the nucleon fields in terms of the nucleus field N , we can calculate the scattering amplitude M :

$$M = f_p \bar{\chi} \chi \bar{p} p + f_n \bar{\chi} \chi \bar{n} n = [Z f_p + (A - Z) f_n] \bar{\chi} \chi \bar{N} N F(q) \quad (2.2.2)$$

$F(q)$ is the q -dependent “form factor”, which encodes the sensitivity of the interaction to the size of the nucleus (i.e. the probing of individual nucleons). If we assume that the WIMP undergoes coherent scattering with the nucleus as a whole, $F(q)$ is approximately the Fourier transform of the nuclear mass distribution. This is known as the Helm form factor [121, 150].

The kinematics of a two-body elastic scatter of a WIMP with a nucleus of mass m_N (and relative velocity v) gives the phase space of final states, and working out the products of the Dirac fields in the non-relativistic limit gives $|M|^2$ from Eq. 2.2.2. Fermi’s Golden Rule then allows us to calculate the differential scattering cross-section:

$$\frac{d\sigma_{\text{SI}}}{dE_r} = \frac{2m_N}{\pi v^2} |M|^2 = \frac{2m_N}{\pi v^2} [Z f_p + (A - Z) f_n]^2 F_{\text{SI}}^2(q) \quad (2.2.3)$$

We have accounted for spin statistics by averaging over initial states and summing over final states. For the case where $f = f_p = f_n$, where the WIMP coherently couples to the entire nucleus and does not resolve individual nucleons,

$$\frac{d\sigma}{dE_r} \sim \frac{2m_N}{\pi v^2} f^2 A^2 \quad (2.2.4)$$

This is the well-known “ A^2 enhancement” for coherent spin-independent interactions that benefits larger nuclei.

By changing the effective Lagrangian, we can study the cross-section for a wide variety of WIMP interactions. For example, for long-range interactions with large momentum transfer, where $g \sim 1/q^2$, there is an enhancement at small recoil energies compared to contact interactions: $d\sigma/dE_r \propto 1/E_r^{-2}$. If we modify Eq. 2.2.1 with Dirac matrix γ^5 so that $\mathcal{L}_{\text{eff}} = g \bar{\chi} \gamma^5 \chi \bar{Q} Q$, we actually get a suppression of the cross-section at low energies: $d\sigma/dE_r \propto E_r$.

It is also important to consider the case where the WIMP interaction depends on the nuclear spin J . A typical Lagrangian for spin-dependent interactions is

$$\mathcal{L}_{\text{eff}} \sim \bar{\chi} \gamma_\mu \gamma^5 \chi \bar{Q} \gamma_\mu \gamma^5 Q$$

This interaction yields the differential cross-section

$$\frac{d\sigma}{dE_r} = \frac{16 m_N G_F^2 (J+1)}{\pi v^2 J} [a_p \langle S_p \rangle + a_n \langle S_n \rangle]^2 F_{\text{SD}}^2(q)$$

where G_F is the Fermi coupling constant, a is the effective coupling for each nucleon, and $\langle S \rangle$ is the average spin contribution for each nucleon.

The SI and SD WIMP-*nucleon* cross-sections are important parameters for comparison across experiments (see Sec. 2.1.3), since different experiments use different nuclear targets. In the SI case, we can simply relate Eq. 2.2.3 to the WIMP-nucleon cross-section σ_p by

$$\frac{d\sigma}{dE_r} = \frac{2m_N}{\mu^2 v^2} \sigma_{\text{SI}} F_{\text{SI}}^2(q), \quad \sigma_{\text{SI}} \equiv \frac{\mu^2}{\mu_p^2} A^2 \sigma_p$$

where μ and μ_p are the reduced masses of the nucleus and proton.

While this section gave an overview of the basic scattering cross-sections, there are countless interactions which may be studied. For a more detailed description of EFT operators and DM interactions, see [7, 97, 100].

2.2.3 Nuclear Recoil Rates

Building a WIMP detector requires not only understanding the probability of interaction, but also an expectation of the WIMP-nucleus scatter rate based on the flux of incoming DM particles. Here we will follow discussions presented in [107] and [150].

The rate of elastic scatters per atomic mass can be estimated using the number density of WIMPs n_χ , the overall scattering cross section σ , and the DM velocity v :

$$R = \frac{n_\chi}{m_N} \langle \sigma v \rangle$$

We average both v and σ over the DM velocity distribution since the cross section is velocity-dependent. Taking the derivative with respect to the nuclear recoil energy and rewriting the DM number density in terms of its mass density, we obtain

$$\frac{dR}{dE_r} = \frac{\rho_\chi}{m_\chi m_N} \left\langle v \frac{d\sigma}{dE_r} \right\rangle$$

To obtain the scattering rate for coherent SI nuclear interactions, we can integrate the WIMP velocity and SI cross section (Eq. 2.2.4) against the velocity distribution $f(\vec{v})$:

$$\frac{dR}{dE_r} = \frac{\rho_\chi}{m_\chi m_N} \int_{v_{\min}}^{v_{\max}} v f(\vec{v}) \frac{d\sigma_{\text{SI}}}{dE_r} d^3v \quad (2.2.5)$$

$$\sim \frac{\rho_\chi f^2 A^2}{m_\chi} \int_{v_{\min}}^{v_{\max}} \frac{1}{v} f(\vec{v}) v^2 dv \quad (2.2.6)$$

We will use the Standard Halo Model with a Maxwellian velocity distribution to approximate the local DM halo, which (in the limit of $v_{\text{esc}} \rightarrow \infty$) is given by

$$f(\vec{v}) = \left(\frac{1}{\pi v_0^2} \right)^{3/2} e^{-|\vec{v}|^2/v_0^2}$$

where $v_0 = \sqrt{2/3} \sigma_v$ is the most probable speed and σ_v is the RMS velocity dispersion. Note that the quantity v is the velocity in the lab frame, boosted using the velocity of the earth relative to the galactic frame.

Using the relation $E = 2\mu^2 v^2/m_N$ (for the WIMP-nucleus reduced mass) and that $v_{\min}$ is the minimum velocity needed for a nucleus to recoil with energy E_r , we get

$$\frac{dR}{dE_r} \sim \frac{\rho_\chi f^2 A^2}{m_\chi v_0^3} \int_{v_{\min}}^{\infty} v e^{-v^2/v_0^2} dv = \frac{\rho_\chi f^2 A^2}{m_\chi v_0} e^{-E_r^2/E_0^2} \quad (2.2.7)$$

Thus, the distribution falls off exponentially with recoil energy, but both the pre-factor and the decay of the exponential depend on the nucleus.

Real detectors have an energy threshold, meaning they can only detect signals down to the level of noise or background. By integrating Eq. 2.2.7 over all energies above a fixed threshold, we can establish the overall integrated detection rate for an ideal detector with perfect efficiency; this is shown in Fig. 2.7. For example, a detector composed of 1 tonne of xenon with a threshold of 10 keV may see only 100 events per year for a 100 GeV WIMP with $\sigma_p = 10^{-45} \text{ cm}^2$ [82].

2.3 Xenon as a Detection Medium

The remainder of this thesis will focus specifically on xenon dark matter experiments and the substantial R&D efforts that aid the success of these large-scale detectors. Therefore,

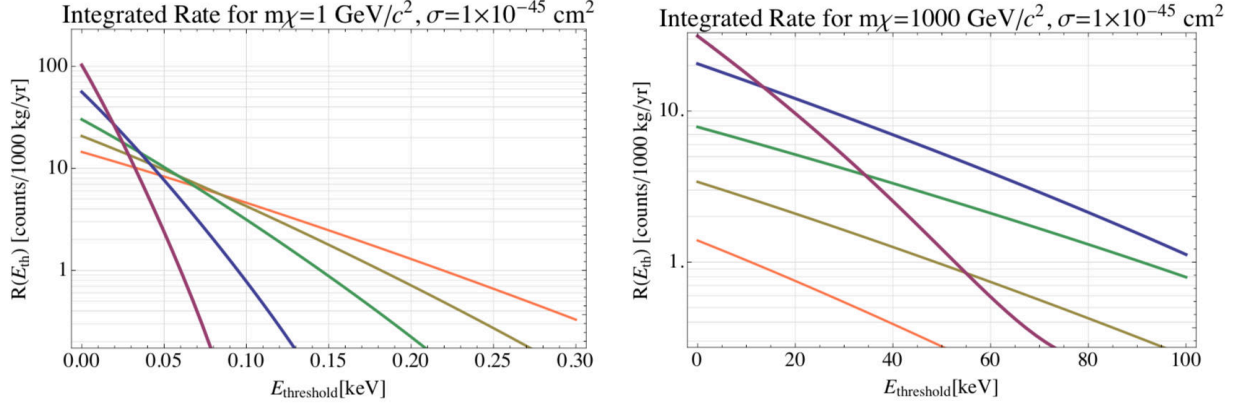


Figure 2.7: Integrated event rates as a function of energy threshold for various detector materials, for 1 GeV (left) and 1 TeV (right) WIMPs with a SI WIMP-nucleon cross-section of 10^{-45} cm^2 : Ne (orange), Si (brown), Ar (green), Ge (purple), and Xe (blue) [82].

some words are in order regarding the importance of xenon as a WIMP detection medium.

Noble elements in general are intriguing detection media, since they have interesting microphysics that gives experimentalists multiple handles for identifying dark matter events (for a more detailed discussion, see Chapter 4). Noble elements are useful for many reasons [39, 53, 82, 205]:

- Their response includes both scintillation photons and ionization electrons, and are transparent to their own scintillation light.
- They offer good discrimination between electron recoils (ER) and nuclear recoil (NR) events, which is useful for separating WIMPs from many backgrounds. This can be done either using the pulse shape (timing) of the scintillation signal or the ratio of ionization to scintillation signals.
- Good position resolution is possible by use of the ionization signal, which facilitates fiducialization (exclusion of backgrounds in the detector periphery).
- Noble elements are chemically inert, meaning they do not readily corrode or react with detector materials. This also means they may be easily purified of electronegative

contaminants using commercial equipment, though removing noble impurities such as krypton remains a challenge.

- Though some noble gases are rarer than others, detector masses are still scalable compared to other technologies (i.e. large dark matter targets are possible).

When it comes to choosing a noble element for a dark matter detector, there are various advantages and drawbacks to each. From the table shown in Fig. 2.8, one can compare some of the physical properties of the noble elements. Heavier elements have higher boiling points (are less cryogenic), however this may lead to a trade off in ease of purification [39]; on the other hand, they have higher light and charge yields.

Property (unit)	Xe	Ar	Ne
Atomic Number	54	18	10
Mean relative atomic mass	131.3	40.0	20.2
Boiling Point T_b (K)	165.0	87.3	27.1
Melting Point T_m (K)	161.4	83.8	24.6
Liquid density at T_b (g cm^{-3})	2.94	1.40	1.21
Volume fraction in Earth's atmosphere (ppm)	0.09	9340	18.2
Cost/kg ^a	\$1000	\$2	\$90
Scintillation light wavelength (nm)	175	128	78
Triplet lifetime (ns)	27	1600	15000
Singlet lifetime (ns)	3	7	<18
Electron mobility ($\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$)	2200	400	low
Scintillation yield (photons/keV)	42	40	30

Figure 2.8: A comparison of physical properties of some noble elements [202].

In addition, the heavier elements have a higher density and atomic mass. High density is crucial for background reduction, since it greatly reduces the penetration depth of γ particles and other radioactivity from external sources and detector materials. In xenon, a typical γ has a mean free path on the order of several cm and a typical radiogenic neutron has a mean free path of ~ 10 cm [14]. This self-shielding allows for a greater sensitive volume after fiducialization [39, 82]. The higher atomic mass is also important, as it greatly enhances the probability of a WIMP-nucleus scatter and improves sensitivity further (recall the A^2 enhancement for SI interactions, Eq. 2.2.4).

Another key difference between the noble elements is their scintillation wavelength. Ne and Ar emit photons with 85 nm and 128 nm wavelengths respectively [53], requiring wavelength shifter to convert scintillation photons into a wavelength that can be detected with good efficiency by modern photosensors. Meanwhile, Xe emits at 175 nm, which is just in the vacuum ultraviolet (VUV) range that is efficiently converted by photocathodes of today's photomultiplier tubes (PMTs).

Xenon, though very expensive, has some clear advantages over other noble elements, and serves as an excellent medium for intermediate-to-high mass WIMPs in particular (note from Fig. 2.7 that Xe loses to Ge at lower energy thresholds). However, efforts to obtain the benefits of multiple noble elements simultaneously have been discussed [149]; specifically, it is possible to dope Xe detectors with Ne or He atoms in sufficiently low quantities to retain the desired Xe properties while increasing signal yields and sensitivity to light WIMPs.

Chapter 3

Edge Reconstruction in the LUX Dark Matter Detector

The **L**arge **U**nderground **X**enon experiment (LUX) is one of the most successful dark matter direct detection experiments to date, having achieved the world's leading exclusion limit in 2016 [21]. It is one of numerous experiments spawned in the wake of the WIMP revolution over the past couple of decades, and has helped advance low-background technologies and calibration techniques for rare event searches.

In this chapter, we will discuss DM search results obtained by the LUX detector, starting with an overview of dual-phase xenon time projection chambers. Complications which arose in the Run 4 analysis, specifically large electric field non-uniformities, as well as efforts to diagnose and calibrate for these issues, will be discussed in detail.

3.1 Dual-Phase Xenon TPCs

A WIMP particle traversing through Xe deposits energy in multiple channels. An interacting particle causes scintillation photons, ionization electrons, and heat to be produced from the event vertex, and a dual-phase time projection chamber (TPC) allows for simultaneous detection of both the photons and electrons. Dual-phase TPCs use both liquid and gas, with

the bulk detection medium being a subset of the liquid volume.

The operation of a dual-phase TPC is depicted in Fig. 3.1. An interacting particle deposits energy in the liquid xenon, which results in the emission of 175 nm ultraviolet scintillation light. This signal is the **S1**, or the “prompt scintillation”, which may be captured by instrumenting the top and bottom of the chamber with photosensors (most commonly photomultiplier tubes, or PMTs).

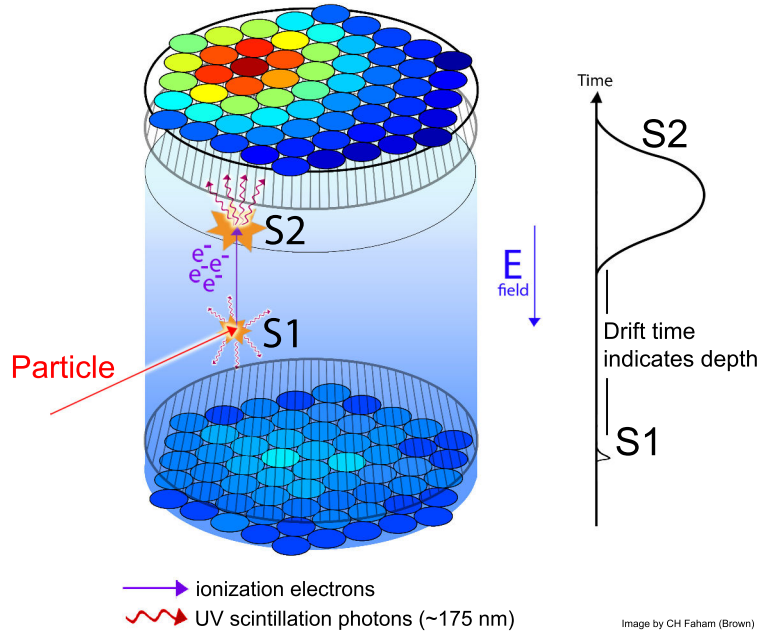


Figure 3.1: An illustration of dual-phase xenon TPC operation, courtesy of Carlos Faham of the LUX collaboration [15].

Electrons emitted due to ionization may also be detected. Instrumenting the top and bottom of the chamber with metal grids, set to high voltage, produces an electric field across the volume of liquid xenon. This “drift field” pulls electrons from the interaction site (which would otherwise just diffuse and/or recombine), and drifts the electrons to the liquid-gas interface. A stronger “extraction field” is applied in this gas region via “gate” and “anode” grids (situated just below and above the liquid-gas interface, respectively), to pull the electrons through the gas gap and produce light through electroluminescence. This secondary signal is called the **S2**.

This procedure provides multiple handles which are needed for event reconstruction:

- **Energy reconstruction:** the measured quantum yields (the S1 photons and, indirectly, the electrons through S2 light) give the energy deposited.
- **Interaction type:** the microphysics of xenon conveniently allows for discrimination of nuclear recoils (“NR”, or WIMP-like events) from electron recoils (“ER” events).
- **XY reconstruction:** the S2 signal creates a hit pattern across the photosensor arrays which can be used to calculate the xy position of the interaction vertex. LUX uses a data-driven maximum likelihood method called “Mercury”, detailed in [25].
- **Depth:** the drift time between the S1 and S2 signals is a proxy for the depth or Z coordinate, provided the drift fields are uniform.

The benefits of using xenon as a detection medium were discussed in Section 2.3. Its self-shielding properties, combined with accurate 3-dimensional position reconstruction, allow for convenient fiducialization, or selection of a “quiet”, low-background subvolume as an active WIMP search region.

There are two important detector parameters which encompass the overall detector response of Xe TPCs: g_1 and g_2 . Assuming that signals are read out from PMTs in units of photoelectrons (phe), these parameters are defined (in units of phe/photon, phe/electron respectively) by

$$S1 = g_1 N_{ph}, \quad S2 = g_2 N_e \quad (3.1.1)$$

where N_{ph} and N_e are the numbers of photons and electrons emitted at the interaction site.

3.2 An Overview of the LUX Experiment

3.2.1 Anatomy of LUX

The LUX detector is a dual-phase xenon TPC, which requires substantial infrastructure in order to maintain stable operational conditions. The experiment is composed of two titanium

cryostats: an outer vacuum vessel and a nested inner vessel (39.75 inches tall, 24.25-inch diameter) which houses the active volume and Xe TPC components. Vacuum insulation of the xenon cryostat is required in order to maintain temperatures of near-cryogenic temperatures (xenon gas at ≈ 2 bar absolute liquefies at ≈ 178 K) [65].

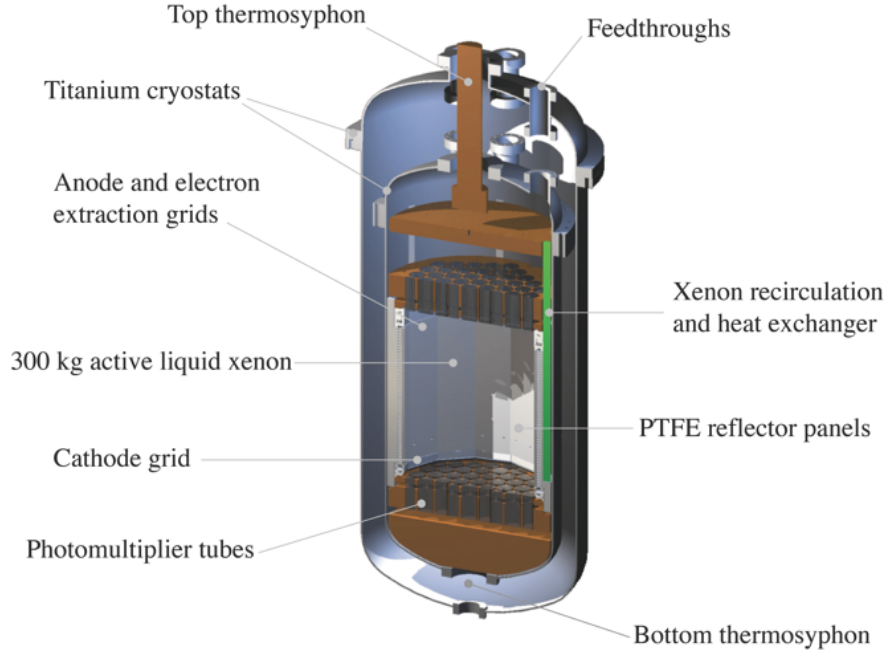


Figure 3.2: A technical cross-section of the LUX cryostat [11].

Thermosiphon technology is used to liquefy the xenon, by means of liquid nitrogen (LN) lines thermally coupled to the xenon space. Insulated stainless steel lines run from condensers immersed in a bath of LN to evaporators (copper cold heads placed in the xenon space). These lines are filled with variable amounts of N_2 , which liquefies above in the condenser, falls down to the evaporator by gravity, and rises back up as gas to the condenser. This cycle transfers heat from the xenon, providing excellent cooling power. A PID loop finely controls the temperature using heaters and thermometers [11].

Xenon must also be recirculated for purification, so as to maximize the electron lifetime by removing electronegative impurities which capture electrons as they drift through the LXe. Recirculation rates must be maximized to purify xenon on convenient timescales. A two-phase heat exchanger is used to improve the recirculation speed by reducing the heat

load of incoming (purified) xenon gas, which also reduces the thermal gradient in the detector and limits the required thermosiphon cooling power and therefore LN consumption [12]. The xenon is pumped from the detector and fed through a heated getter purifier for removal of electronegative impurities before returning through the heat exchanger.

The wall of the TPC is composed of polytetrafluoroethylene (PTFE) reflector panels, which form a dodecagonal prism enclosing 300 kg of xenon. PTFE is used to maximize light collection, since it has excellent reflective properties in liquid xenon [111, 167] and is a relatively clean, low-outgassing material.

The top and bottom of the TPC are each instrumented with an array of 61 2-inch Hamamatsu R8778 PMTs, giving 122 PMTs in total. A series of parallel-wire stainless steel electrode grids are placed as follows: a cathode grid is located just above the bottom PMT bank, while the gate and anode are placed just below and above the liquid-gas interface respectively. The gate and anode produce a strong extraction field across the gas gap, allowing for optimal S2 production.

To help with temperature control, large copper structures connected to the thermosiphon system are placed above the top PMTs and below the bottom PMTs; these provide additional γ shielding as well. The entire detector (including the outer vessel supports) is surrounded by a 7.6-m diameter, 6.1-m high water tank for shielding against γ and neutron backgrounds from cavern radioactivity. This water shield also serves as a muon veto through the tagging of Cherenkov radiation with 10-inch water PMTs.

For a more thorough discussion of instrumentation and electronics, see [11] and [15].

3.2.2 The Sanford Underground Research Facility (SURF)

As is common with low-background experiments, the LUX detector was operated underground in order to shield it from cosmic rays. The LUX experiment was operated at the Sanford Underground Research Facility (SURF) in Lead, South Dakota, at the 4850-foot level within the former Homestake gold mine.

The LUX detector was partially assembled above ground in the Surface Lab, including



Figure 3.3: A panoramic view of the LUX water tank in the Davis Cavern.

the detector subsystems and inner and outer cryostats. The TPC was then transported underground in 2012, when it was installed in the Davis Cavern. The cavern, about 10.5 m long, 18 m wide and 12 m high, was named after Ray Davis, who carried out his famous solar neutrino experiments there between 1970 and 1994 [11]. The cavern has both an upper and lower level, the upper deck allowing access to the detector breakout system and housing a control room for scientists.

Workers and scientists access the 4850 level of the mine via a hoist conveyance in the Yates Shaft (affectionately termed “the Cage”), which also served as the method for delivery of the LUX detector during TPC transport.

3.2.3 Background Mitigation and Estimation

In a search for rare nuclear recoil (NR) events such as a WIMP scatter, the ultimate goal is to suppress interfering background events as much as possible. Some backgrounds may be discriminated during analysis, while others are indistinguishable from WIMP interactions.

Through careful screening of detector materials [10, 26] and extensive shielding of the fiducial xenon volume, WIMP-like events may be highly suppressed. The background component that dominates the WIMP search region consists of electron recoil (ER) events, which are caused by incident γ or β particles scattering off atomic electrons. The low-energy ER

backgrounds of interest come mostly from four sources [14]:

1. ^{85}Kr , ^{39}Ar or radon daughter contaminants in the liquid undergoing β decay where the γ escapes (is not detected).
2. X-rays from ^{127}Xe electron capture decays where the γ escapes (is not detected).
3. ^{37}Ar contaminant from exposure to laboratory air, producing electron capture decays at 2.8 keV in the fiducial volume.
4. Compton scattering of γ -rays from radioactive detector components.

The intrinsic component of low-energy ER events from radioisotope decays homogeneously mixed within the Xe target is of major concern. β and X-rays are produced and absorbed within a few mm of the decay site, resulting in small energy depositions localized in the fiducial volume. This component is mitigated by removing noble radioactive contaminants such as ^{85}Kr and ^{39}Ar through charcoal-based chromatographic separation (an alternative to cryogenic distillation) [24].

Excessive γ backgrounds observed in the detector, particularly from components in the bottom region (the PMT–copper assembly) [14], are the result of nuclear de-excitations from the ^{238}U decay chain, the ^{232}Th decay chain, and ^{60}Co . Resulting low-energy Compton scatters may bleed into the WIMP search region. Of less concern are external γ from the surrounding cavern walls, which are suppressed below significance by the 300 ton water tank.

While ER backgrounds may be discriminated in analysis, NR backgrounds must be well-estimated and well-suppressed for a successful WIMP search. Some components are negligible over the entire LUX run: random coincidence of “fake” S1 (from PMT dark noise) and S2-only signals, neutrino–nucleus scattering, and background neutrons sum to give ~ 1 event/year [13, 21].

The muon and neutron (cosmic and induced) fluxes at the 4850-foot level of the Homestake mine have been well-modeled and characterized [14, 63, 106, 157, 159]. Cosmic ray muons are highly suppressed by the mile of earth, however high energy μ ($E \approx 321$ GeV)

can still penetrate down to the cavern and induce high-energy neutrons ($E > 10$ MeV) in the cavern rock or in the water tank. The overall rate of this is still quite small: ~ 0.1 WIMP-like events in 100 kg years. There is also an external neutron flux dominated by fast neutrons ($E > 1$ MeV) from the surrounding rock/concrete of the cavern, due to spontaneous fission of ^{238}U and (α, n) neutrons from the ^{238}U and ^{232}Th decay chains. These are suppressed by the water tank to a negligible 10^{-16} n/yr incident on the detector.

Another source of backgrounds (and perhaps the most difficult to characterize) comes from the periphery, near the PTFE detector walls. Here, the signal distribution differs from the bulk for a number of reasons which may cause leakage of the events into the WIMP search region: incomplete charge collection, electric field-fringing (non-uniformities), and poor position reconstruction resolution. Additional WIMP-like NR events caused by the decay of radon progeny from the PTFE surface is of concern in this region; in LUX their rates have been assessed through the associated spectrum of high-energy α signals. Such backgrounds will be discussed in detail in Sec. [5.1](#).

3.3 Detector Calibrations

Before either claiming discovery or setting an exclusion limit for WIMP scatters, the detector response must be characterized with calibration sources. Not only does calibration set the energy scale for different kinds of particle interactions, but it also allows for the correction of systematics such as signal variation throughout the detector.

There are two main types of calibration sources used in LUX: electron recoil (ER) and nuclear recoil (NR) sources. These may be further subdivided into different microphysics models, however for the purposes of a WIMP search these two main categories are the most convenient since they may be discriminated by their charge-to-light ratio.

3.3.1 ER Calibrations

For the ER calibration shown in Fig. 3.4, LUX used a number of internal and external sources. An external ^{137}Cs source was used to generate a 662 keV γ . Of similar energy was the intrinsic detector background from ^{214}Bi , providing a 609 keV γ .

Mono-energetic lines from various Xe isotopes (^{127}Xe , ^{129m}Xe , and ^{131m}Xe) were present early in the first underground run due to the cosmogenic activation on the surface. These proved to be very useful, as they span a wide energy range (186 eV – 409 keV, including associated γ) and allowed for a dedicated low-energy calibration using the X-rays from various electron capture modes of ^{127}Xe [23].

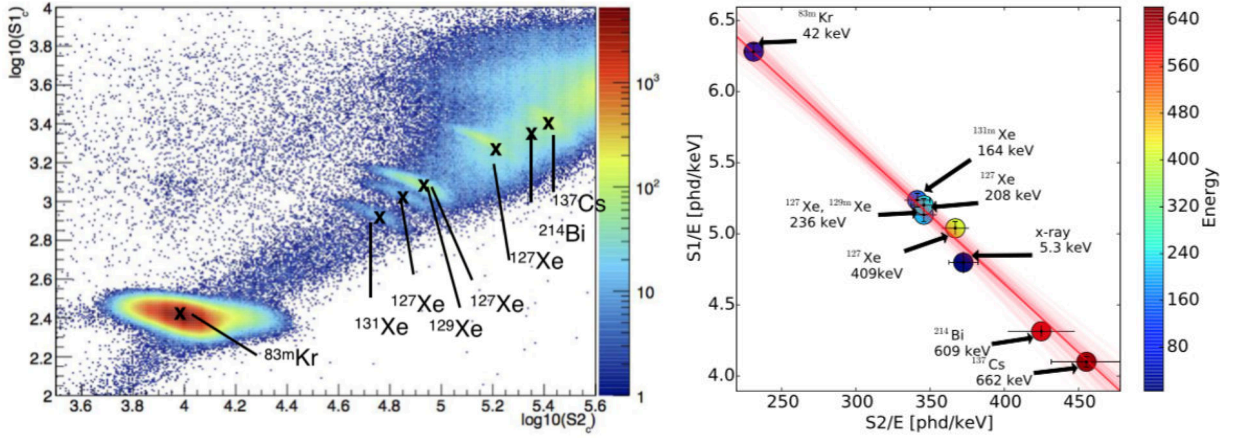


Figure 3.4: (Left) A variety of ER calibration populations in corrected S1-S2 space. (Right) The LUX Doke analysis using various sources to calibrate the ER energy scale. From [29].

LUX used two injected ER sources which proved to be especially useful for separating different detector effects. The first was tritium, ^3H , dissolved uniformly into the LXe of LUX by injection of tritiated methane, CH_3T . This host has been shown to be removable via standard getter purification and minimally diffusive into detector components, and thus serves as a clean carrier of tritium activity [17]. Furthermore, it is important for obtaining an ER calibration band in the WIMP search energy range (see Fig. 3.6), since it is a β emitter with a continuous low-energy spectrum and a mean energy of 5.6 keV.

The other injected source is ^{83m}Kr , which is precisely dosed from a charcoal mediator

doped with ^{83}Rb into the path of Xe gas [28]. As can be seen from Fig. 3.5, this source evenly mixes with the LXe. Since the mono-energetic lines associated with krypton are spread throughout the detector, the spatial variations in the detector response can be calibrated by breaking the detector into voxels. A 3-dimensional map of the average krypton S1 signal gives the variation in light collection efficiency across the detector, therefore providing S1 corrections. The S2 signal is more complicated, involving:

- xy -dependent corrections due to non-uniformity of electron extraction at the liquid-gas interface (including grid sag/deflection, liquid level or pressure variance, and varying light collection in the gas gap).
- z /drift time-dependent corrections due to drifting electrons being eaten by impurities.

Correction maps are therefore also generated for the S2 signal from krypton, though the electron extraction and electron lifetime corrections are done separately since the actual production of the S2 is localized to the gas gap.

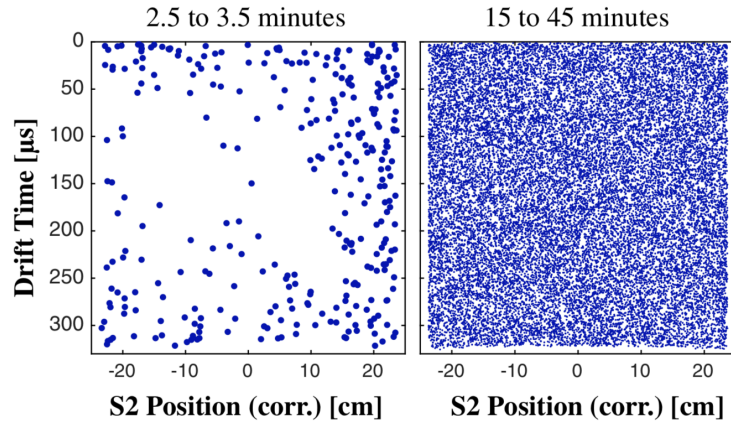


Figure 3.5: The mixing of ^{83m}Kr over time in LUX. The event position is projected on a plane such that movement from right to left leads away from the Kr inlet. Clockwise mixing is observed, with maximal mixing occurring in under an hour [28].

The importance of using both of these injected sources was emphasized in Run 4 where, as will be discussed in Sec. 3.5, non-uniformities in the electric drift fields became a major

concern. Large field variations result in physical differences in the light and charge yields across the detector *in addition* to the normal geometric effects already discussed. While the low-energy events of tritium have a very weak field dependence, ^{83m}Kr decays in two steps (32.1 and 9.4 keV) which provides two higher-energy S1 signals. The ratio of these signals results in a quantity that depends *only* on the applied field. Thus, leveraging both sources allowed for both field-independent and field-based calibrations during Run 4 [21].

Using the mono-energetic lines from the various ER sources, a “Doke analysis” was performed to quantify the efficiencies of the LUX detector and produce a combined energy scale (CES) for ER events (Fig. 3.4). This method improves energy resolution by leveraging the anti-correlation of the S1 and S2 signals caused by electron recombination and taking a linear combination of S1 and S2 signals to calculate the deposited energy; it also gives g_1 and g_2 , which allows for the direct measurement of light and charge yields. This technique will be discussed in greater detail in Sections 4.1.2 and 7.4.3.

3.3.2 NR Calibrations

Nuclear recoils require a separate calibration from ER interactions not just because they experience a quenching of the overall quanta, but because they present a characteristically different charge-to-light ratio (see Sec. 4.1 for a discussion of the underlying physics).

To calibrate the NR response of LUX, multiple external sources were used. In Run 3, neutron sources Americium-Beryllium (AmBe) and ^{252}Cf were used to generate an NR band for assessing discrimination power (Fig. 3.6), as well as for obtaining absolute signal finding/classification efficiencies through hand-scanning of events [13].

However, given the uncertainties in their deposited energy, these sources provide neither a true NR energy scale nor a means of measuring absolute light/charge yields from the S1/S2 signals. The LUX collaboration therefore implemented a new technique for NR calibration: a deuterium-deuterium (D–D) fusion source of mono-energetic neutrons, collimated through the surrounding water tank toward the middle of the TPC drift region. This source produces neutrons of known initial energy (2.45 MeV) whose deposited energy may be

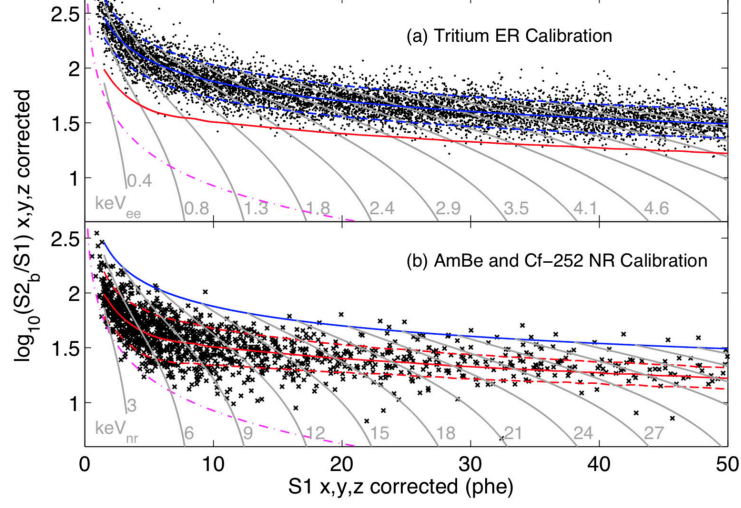


Figure 3.6: Run 3 calibration events plotted in terms of the charge-to-light ratio, along with the resulting ER (top, blue) and NR (bottom, red) calibration bands [13].

reconstructed through the scattering kinematics; in addition, the pathology of mis-identified multiple scatter sub-cathode events (due to missing S2 signals) is largely removed [27].

Using the precisely measured g_1 and g_2 parameters, the absolute light and charge yields for NR energies down to 0.7 keV were measured *in situ* for the first time. These measurements

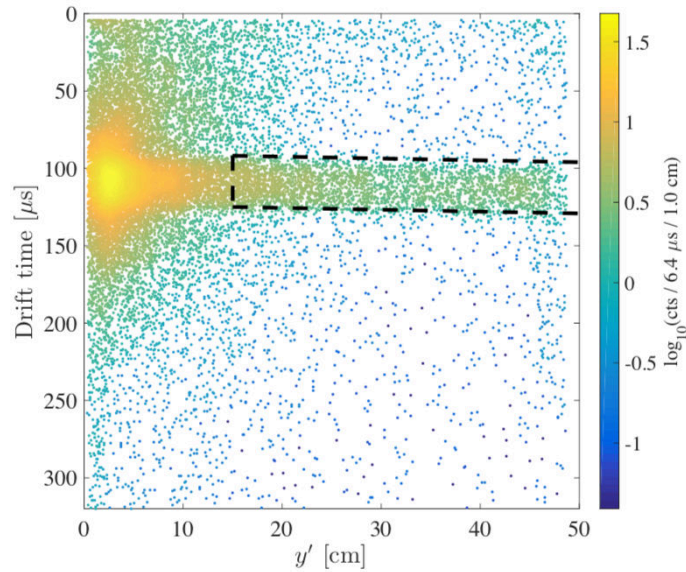


Figure 3.7: Neutron single scatter events for the Run 3 calibration, with the black box indicating the approximate location of the “beam purity” cut [27].

provided improved models for estimating low-energy background scatters and refined NR signal detection efficiency estimates. Single scatter neutron events passing a “beam purity” cut (Fig. 3.7) were used to generate a new NR band for use in the WIMP search profile likelihood analysis [29].

3.4 Results from the Complete WIMP Search

The LUX detector performed two WIMP search runs underground: Run 3 (95 live-days) in 2013 and Run 4 (332 live-days) in 2014–2016. Calibration data, including source injection acquisitions, were collected intermittently throughout both runs for consistent tracking of the detector response. For both runs, periods of unstable detector conditions or low electron lifetime (i.e. low purity) were excluded from the remaining background livetime and clean single-scatter events were used in the final profile likelihood analysis.

The final WIMP-search events for Run 4 are shown in Fig. 3.8. Note that a population of fiducial events persists in the nuclear recoil band, particularly at low S2; most of these are

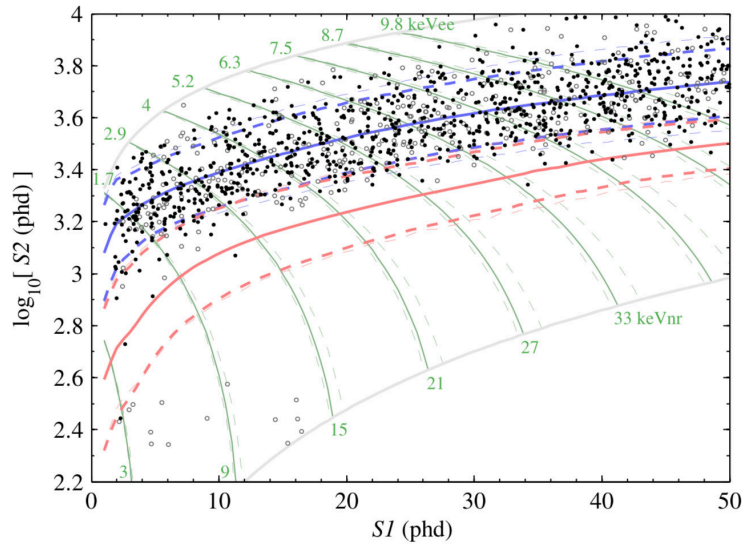


Figure 3.8: Run 4 fiducial single scatter events meeting all selection criteria. Shown are calibration bands for ER (blue) and NR (red), fiducial events (black), and fiducial events within 1 cm of the fiducial boundary (unfilled circles) [21].

near the edge of the fiducial volume, indicating they likely come from charge suppression of radon progeny decay at the detector walls (including ^{206}Pb nuclei from ^{210}Po decay).

The most current LUX DM limit will be discussed here, which combines the results from both runs. However, the two runs ultimately required very different treatment due to the aforementioned drift field non-uniformities. For Run 3, a single exposure with a single set of Xe response models was used for the duration of the run with a constant fiducial Xe mass of 118 kg. For Run 4, this treatment is impossible given the large dependence of the physics on both event position and time during the run.

Run 4 is therefore broken into 16 separate exposures: 4 date bins dividing the duration of the run, each with 4 drift time bins. The bins are broken up this way since the field varies most significantly in these two parameters. Furthermore, each exposure uses separate Xe response models (i.e. calibration bands) as well as separate electric field magnitudes. These drift fields are obtained from COMSOL models and independently cross-checked through fitting of field-dependent signal amplitudes predicted by NEST simulations [21].

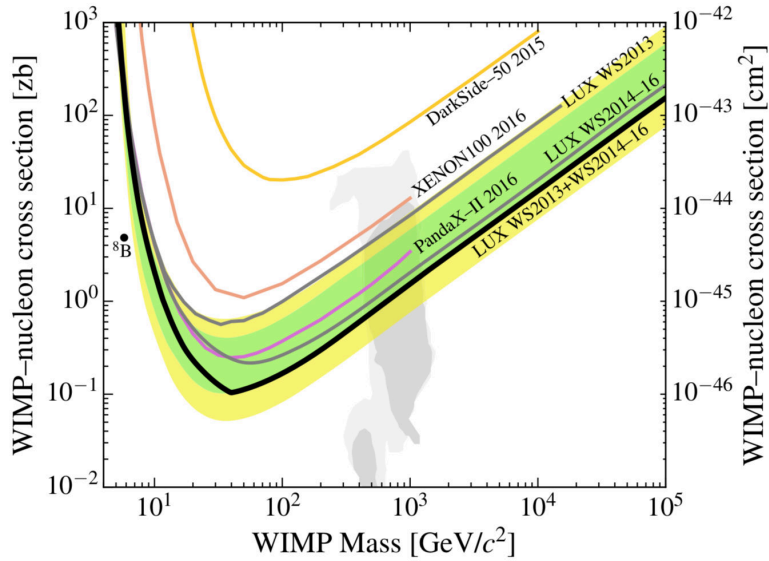


Figure 3.9: The SI WIMP-nucleon cross-section exclusion limits set by Run3, Run 4 and the combined LUX exposure. Also shown is preferred cMSSM phase space (grey) [21].

To perform a combined WIMP search analysis, Run 3 is added as a 17th exposure to the

16 bins of Run 4. These exposures each have their own signal and background models, which are used to construct the probability density functions (PDFs) used to test DM hypotheses with the profile likelihood ratio (PLR) method. This is done over a range of WIMP-nucleon cross-sections for various WIMP masses. Systematics in the detector response are accounted for by including them as nuisance parameters, which are constrained using sideband measurements. The resulting p values are consistent with the null hypothesis, and so an exclusion limit is calculated at the 90% confidence limit (Fig. 3.9).

3.5 Electric Field Non-Uniformities in Run 4

Between Run 3 and Run 4 exposures, the LUX grids were subjected to a conditioning campaign in order to raise their maximum operational voltages, thereby increasing extraction fields and the electron extraction efficiency. The anode, gate, and cathode grids were held at voltages just above that needed to create sustained discharge for multiple days in cold xenon gas. While the campaign successfully raised the maximum extraction field from 2.9 kV/cm to 3.5 kV/cm and extraction efficiencies from 49% to 73% [21], the PTFE panels making up the TPC walls were unexpectedly charged.

From studies of calibration data, it became clear that electrons from events at high drift time (or lower z -coordinate) were exiting the liquid at smaller radii due to deviations in the electron trajectories. The time-, depth-, and azimuth-dependence of this is consistent with a non-uniform time-varying negative charge density in the PTFE panels. It is understood that coronal discharge in the gas created VUV photons which liberated electron-hole pairs in the PTFE [242]. Furthermore, it is well known that PTFE has high resistivity and can maintain substantial charge [108, 139], and that under an electric field holes have a higher mobility than electrons, resulting in a net buildup of negative charge [208, 243]. The behavior of charges in PTFE is well-studied at room temperature [117, 246].

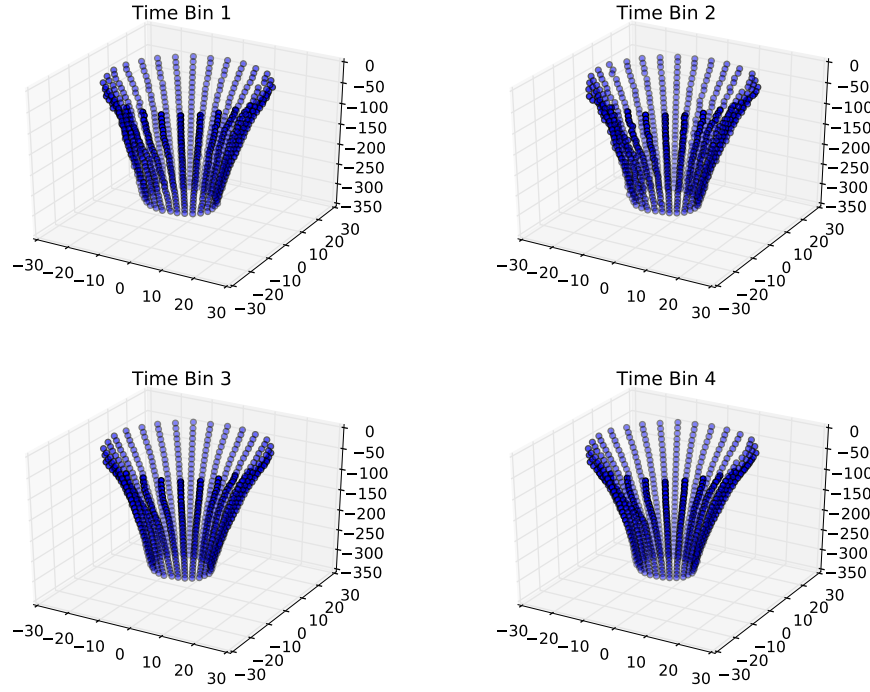


Figure 3.10: The observed location of the detector wall in S2 coordinates, using reconstructed positions of localized wall backgrounds (as in [67]), throughout various “time bins” of Run 4. The z axis here (negative drift time) serves as a crude proxy for depth.

The resulting field effects introduced a number of complications to the Run 4 analysis:

- There is no longer a simple scaling between drift time and z -coordinate (i.e. electrons now have a non-vertical trajectory, as well as a varying drift velocity).
- The xy -position reconstruction is now heavily dependent on the depth.
- Position-dependent detector response calibrations (due to variations in light collection, etc.) are now entangled with the field variations.
- Comparison with existing Xe physics models (i.e. NEST) requires an understanding of the field profile, as light and charge yields in Xe are field-dependent.

There are numerous ways to approach these issues. Such decisions are informed by characterization of the field profile, and thus an electrostatic model was developed for the

LUX detector using COMSOL Multiphysics® software. A simplified 3D model of the LUX TPC was used with the PTFE walls split into 42 “charge tiles” (6 angular $\times$ 7 vertical). These charge tiles are unit vectors with which the overall charge distribution is built. Simulations are iteratively performed with a given charge model to drift electrons through the detector, and observed S2 coordinates are compared with krypton data using a Metropolis-Hastings algorithm [18]. A simulated field map is then frozen from a converged charge model. This process is repeated for krypton datasets throughout Run 4.

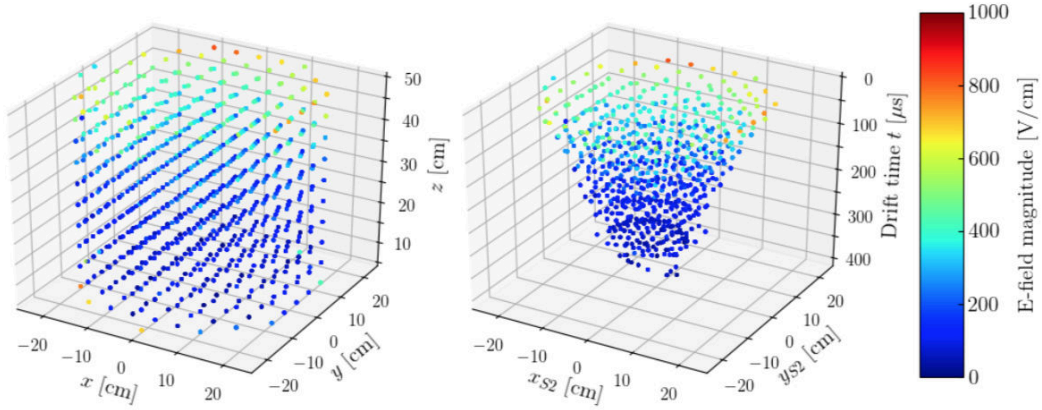


Figure 3.11: An example COMSOL field map, with starting vertices in “real space”(left) and resulting observed S2 coordinates (right). The color map indicates field magnitude. [18]

These field maps became an important tool in the Run 4 analysis, as they give resultant “S2 space” vertices from a set of “real space” vertices (see Fig. 3.11). However, in order to develop corrections and study field effects, we had to develop tools that could apply these field maps to arbitrary data.

3.6 JPM – Mapping from Observables to Reality

Given the scope of the Run 4 field non-uniformities, it was necessary to develop a comprehensive correction algorithm which combines all available tools at the disposal of LUX.

The algorithm I have developed (**J**acob’s **P**osition **M**apping, **J**acob’s **P**osition **M**agic, or **JPM**) is a product of extensive efforts to map from so-called “S2 coordinates” (reconstructed

xy and drift time coordinates) to “real coordinates” (true xyz space).

Prior to the development of COMSOL field maps for Run 4, there were attempts to perform xy corrections entirely using a krypton-based binning technique (“Delensing”), which will be discussed in 3.6.2. However, these corrections are limited, as they are not field-based and therefore do not account for large-scale deviations in the electron trajectory in both the radial and z directions.

Thus, the idea was born to merge techniques into a two-step algorithm: interpolating “rough real space” coordinates from the COMSOL field maps, then applying a set of refining Delensing corrections to map to “real space” coordinates. Both of these steps will be discussed below.

3.6.1 Exploring Interpolation Methods for the Field Maps

The COMSOL field maps discussed above include a grid of drifted electrons, with the following information: real-space xyz coordinates of the initial electron vertex, the electric field at that position, and the final S2 coordinates ($x_{S2}, y_{S2}, \text{drift}$) of that electron after drifting.

In order to calculate either the electric field magnitude or the corresponding S2-space position for an arbitrary event, an interpolation algorithm is needed for doing a weighted mapping between field map vertices. Various interpolation methods were studied, as is discussed below.

3.6.1.1 Trilinear Interpolation

One of the simplest and fastest algorithms for interpolating on a regular lattice of points is trilinear interpolation, or linear interpolation on a 3-dimensional grid. Given a set of nearest neighbors, one can use the distances between the subdividing planes to interpolate a value at an arbitrary point within the volume formed by the neighbors.

The procedure is shown in Fig. 3.12, which illustrates how the distances to opposite corners determine the weighting of the values at those corner points. It is essentially a linear interpolation of two bilinear interpolations (for the front and back faces of the cubic volume)

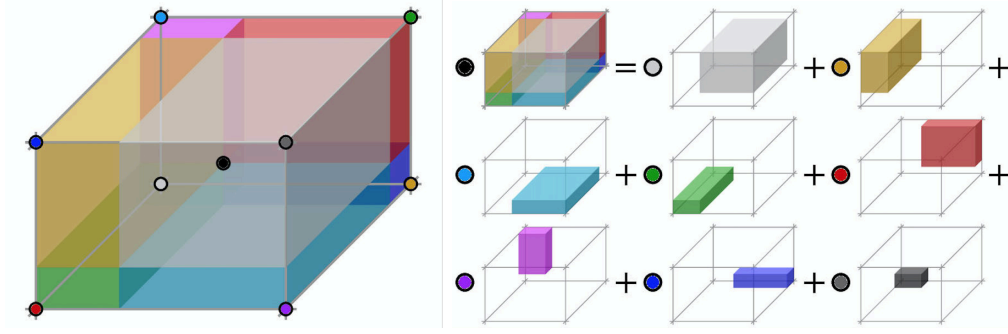


Figure 3.12: An illustration of trilinear interpolation, courtesy of user “Cmglee” on Wikipedia Commons. The colored dots indicate the values to be interpolated and the colored cells indicate the distance weighting for that value.

[207]. For a unit cube centered at the origin, the equation for this procedure is [66]:

$$\begin{aligned}
 V_{xyz} = & V_{000} (1 - x)(1 - y)(1 - z) + V_{100} (1 - y)(1 - z) + V_{010} (1 - x)y(1 - z) \\
 & + V_{001} (1 - x)(1 - y)z + V_{101} x(1 - y)z + V_{011} (1 - x)yz \\
 & + V_{110} xy(1 - z) + V_{111} xyz
 \end{aligned}$$

This method has been used to interpolate with LUX field maps to map simulated data from real space to S2 space, since it only works for uniformly-spaced lattices. However, we would like an algorithm which allows us to investigate randomly-distributed detector data in real space coordinates, i.e. map from S2 space to real space.

Furthermore, this algorithm is constrained to the nearest neighbors in a cubic region, which results in highly discrete results. The algorithm also fails if any neighboring lattice points are missing, which is common near the edge of the field maps.

3.6.1.2 Inverse Distance Weighting (Shepard’s Algorithm)

Given that we want to construct a mapping from S2 space to real space, it is necessary that our interpolation be able to handle a non-uniform scattered distribution of events.

One of the simplest non-intensive algorithms in this case is a simple inverse distance weighting (IDW), or Shepard’s algorithm. This technique has well-known uses in geographic

information systems, computer graphics, and other applications of spatial data sampling [3, 144, 151]. To interpolate a functional value $f(\vec{x})$ at an arbitrary point P using this method:

1. The distances from P to its neighbors (the interpolation points) are calculated using some distance metric d .
2. In the case of a “modified” Shepard’s algorithm, the list of neighbors may either be truncated to some number of nearest neighbors N or only neighbors within radius R .
3. The interpolated value of f is then calculated from a sum weighted by an inverse power of the distance metric, thereby weighting closer neighbors more heavily:

$$f(\vec{x}) = \frac{\sum_i d_i^{-p} f(\vec{x}_i)}{\sum_i d_i^{-p}} \quad (3.6.1)$$

where we sum over neighbors indexed by i and p is an integer weighting power. Note that the function f depends on multiple coordinates.

However, even defining a distance metric in our domain of “S2 space” is non-trivial. Since drift time is not actually a spatial measure, but a scaled proxy for z (in uniform electric fields), we must scale the drift time by a velocity factor when defining our metric:

$$d = r_{S2} = \sqrt{(x - x_{S2})^2 + (y - y_{S2})^2 + v_{\text{drift}}^2 (\text{drift} - \text{drift}_{S2})^2} \quad (3.6.2)$$

Without such a scaling, interpolation results are greatly skewed, since the interpolation is performed in a highly ellipsoidal volume in S2 space. This method for calculating the interpolation distance is shown in Fig. 3.13.

This metric has a built-in systematic, however. There is large variance in the drift velocity scale factor, since electric fields are highly non-uniform. Using local field information from the COMSOL models to derive a position-dependent velocity factor has been considered, however this is non-trivial to achieve, given that the drift velocity has to be integrated along the entire electron trajectory. The simplest solution is therefore to use a mean drift velocity,

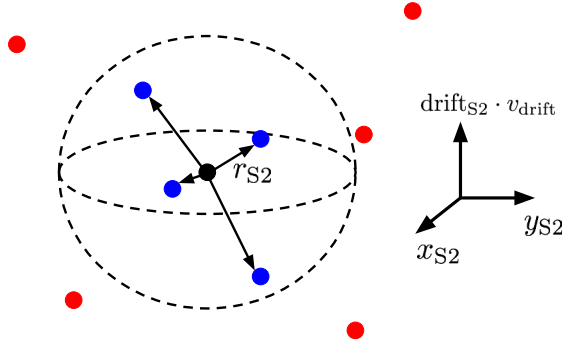


Figure 3.13: An illustration of IDW interpolation in S2 space, including field map neighbors (blue dots) in a certain interpolation radius (dotted sphere).

and subsequently treat edge effects through additional krypton-based corrections (such as the Delensing algorithm, which will be discussed in Sec. 3.6.2).

To choose an “interpolation radius”, the nearest neighbor S2 distance is plotted for many krypton events, and a natural cutoff value is found which separates the bulk events from outer wall events which are likely mis-reconstructed. All neighbors contained within a certain radius are used in the interpolation, and events with no sufficiently close neighbors are handled as an exception case.

We also must choose an appropriate weighting power p , which effects the range of the interpolation. If the entire field map were included in the interpolation (order $\sim 10^5$ points), increasing this power would give greater influence to the closest points, giving results which are tiled or tessellated like a Voronoi diagram [48, 144, 145]. Given that we are only interpolating with the closest neighbors, we apply a power of $p = 1$ to smoothly average over these points.

Since the COMSOL field maps provide the electric field at each electron vertex, we can use the IDW method to interpolate the local electric field for an arbitrary event. This serves as a cross-check the interpolation algorithm, since we can directly compare the interpolated electric fields for krypton events with the COMSOL field model profile (see Fig. 3.14). In the bulk, there is very good agreement with the COMSOL maps. Horizontal striations of

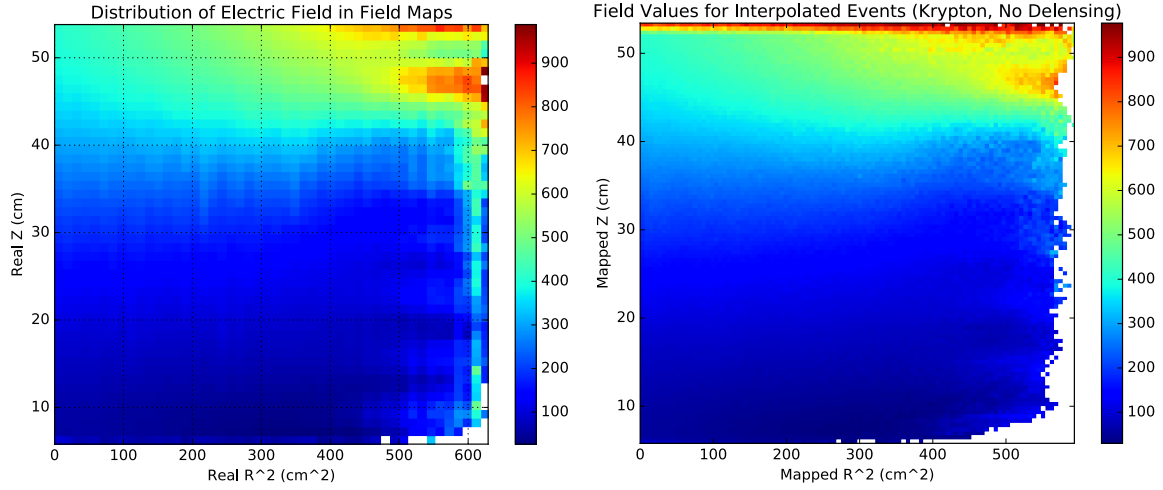


Figure 3.14: (Left) Color map of the electric field profile (in V/cm), plotted directly from the COMSOL field maps. (Right) The interpolated field values for randomly distributed krypton events mapped to “rough real space”.

higher field due to the discrete charge tiles in the COMSOL model can be resolved in both distributions, even at higher radius. There are certainly edge discrepancies, particularly at the liquid surface ($z \approx 53$ cm), where the interpolated field is higher. At large r^2 there appears to be an inefficiency of events, which is caused by both inward-clustering effects and exception cases near the walls.

This interpolation method certainly has shortcomings. It is well-known that for $p > 1$ a “flat spot” (null derivative) occurs at each data point [102, 144] and that the method tends to produce “bulls-eye” or “duck-egg” patterns at the interpolation points [3]. However, IDW may produce comparable results to more robust yet cumbersome algorithms using radial basis functions or the Kriging method, and is especially convenient for sparse datasets [48, 154].

3.6.1.3 Multilinear Extrapolation

A weakness in the previous interpolation method is that it inherently fails for events at the edge of the detector, due to field-based systematics and missing field map points. Another algorithm was considered to better treat these peripheral events: multilinear extrapolation.

By extrapolating from the field map points rather than interpolating, edge events would hopefully fill in “holes” in the field maps and soften the inward-clustering effect of IDW.

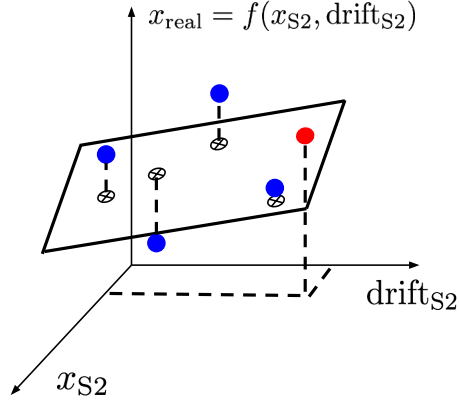


Figure 3.15: An example planar fit simplified to two S2 coordinates, to extrapolate the red point at arbitrary S2 coordinates from the blue field map points.

The algorithm works as follows for calculating a real coordinate x_{real} :

1. If the nearest field map neighbor is outside a pre-defined interpolation radius, use the extrapolation method; otherwise, use the IDW method as previously described.
2. Fit a planar function of S2 coordinates f_x through the interpolation values $x_{\text{real},i}$ of the n closest field map neighbors and extract the fit parameters:

$$x_{\text{real}} = f_x(\text{S2}) = A \cdot x_{\text{S2}} + B \cdot y_{\text{S2}} + C \cdot \text{drift}_{\text{S2}} + D \quad (3.6.3)$$

3. Evaluate the resulting fit function at the S2 space coordinates to extrapolate the real space coordinate.

As discussed in the previous section, an interpolation radius is determined from the bulk krypton data. However, rather than simply throwing an exception, edge events are now mapped to real space using the above extrapolation method.

The performance of this method is illustrated in Fig. 3.16. It is clear that this gradient fitting method actually *accentuates* the “scallop” in the (r^2, z) distribution, rather than

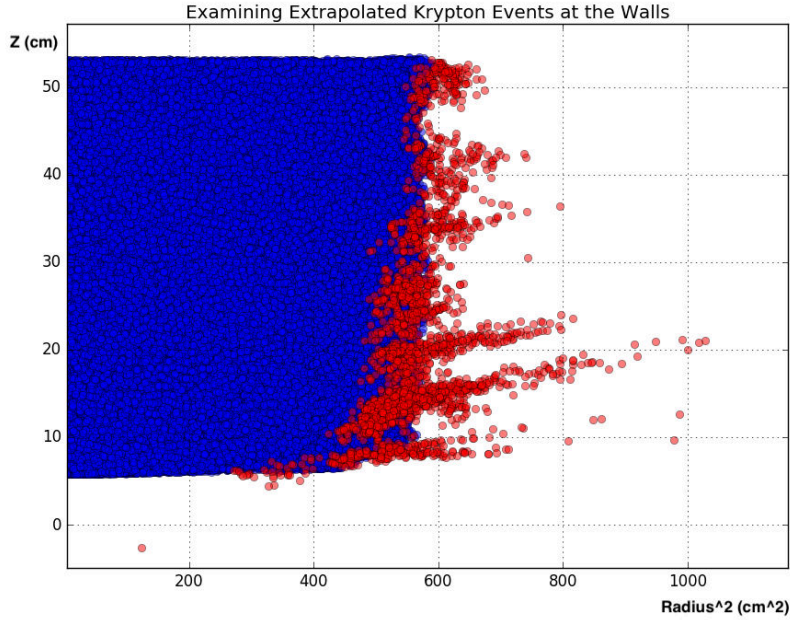


Figure 3.16: A sample krypton dataset mapped to real coordinates using a combination of interpolation and extrapolation, based on neighbors within the interpolation radius.

filling in the gaps. The scallops, which are thought to be caused by the discrete PTFE charge tiling in the COMSOL model, are present where the field is the most non-uniform. Locally fitting this 3-dimensional function is therefore understandably difficult. Since this method fails to achieve its main goal of better reconstructing edge events, and it appears to add unphysical smearing, it was not implemented in the final JPM algorithm.

3.6.2 The Delensing Method

As previously discussed, krypton serves as a highly uniform calibration source that mixes evenly with liquid xenon over relatively short timescales. Furthermore, krypton produces a unique set of signals which allows for easy selection and background exclusions [28].

Let us presume that we have mapped krypton data from S2 space to a “rough real space” using an interpolation algorithm discussed above. Given that krypton is physically uniform, any density variations in the resulting distribution encodes systematics of the interpolation algorithms or the field maps themselves. Thus, the mapping which levels the distribution

serves as a flat-fielding correction.

Such a correction is created by tessellating the krypton distribution into spatial cells of equal density. This generates a set of non-uniform correction bins which may be mapped to a set of uniformly-spaced bins whose outermost boundary is defined by the physical detector geometry. The correction bins essentially provide scaling factors by which to adjust the spatial coordinates for a given event (see Fig. 3.17 for a simple demonstration).

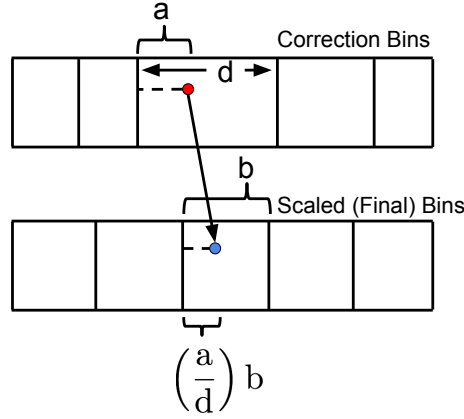


Figure 3.17: A simple diagram of bin scaling corrections in one dimension.

Since the end goal of this procedure is to undo the lensing effect of the non-uniform fields on drifting electrons, this algorithm is called “Delensing”. The following procedure is done to generate Delensing correction tables:

1. Load krypton data for a given time range (~ 1 month) during Run 4.
2. Map krypton event positions to “rough real space” using the preferred interpolation algorithm with the LUX field maps.
3. Generate a set of equal-density, non-uniform “Delensing bins” in the z dimension.
4. Break up the distribution into uniform z slices, and in each slice generate Delensing bins in the ϕ dimension (using periodic boundary conditions).
5. Break up the distribution into pie slices in (ϕ, z) , and for each pie slice generate Delensing bins in the r^2 dimension.

6. Record tables of correction values to a XML file (“Extensible Markup Language”, a common format used by LUX for data processing); this includes a vector of bin edges for z , a 2-dimensional array for ϕ , and a 3-dimensional table for r^2 .

These correction tables are later processed and applied to arbitrary datasets, in order to produce full spatial corrections as a function of (z, ϕ, r^2) . Just as field maps were produced for datasets throughout Run 4 to account for any temporal variations, Delensing corrections are generated for each field map and its corresponding krypton datasets, so as to maintain consistency and accuracy.

There are some subtle but important points regarding the boundary conditions of the Delensing algorithm. Since the goal of the Delensing correction is to improve accuracy near the detector walls, it is important to carefully define the “wall” of our distribution. To do this, localized wall events are collected from throughout Run 4 (see Fig. 3.10) and mapped to “rough real space” along with the krypton. The spread in this data is almost purely due to position reconstruction error, and therefore we use the median r^2 of this distribution to define the krypton distribution boundary. Any events that live outside this wall boundary are linearly extrapolated away from the outermost r^2 bin, thereby preventing leakage of mis-reconstructed events into the bulk Xe.

Delensing therefore maps this wall definition in “rough real space” to the geometric boundary of the LUX detector. The mapping of the wall data distribution to the physical detector wall is shown in Fig. 3.18; the mean r^2 of the resulting Delensed wall distribution corresponds to the mean radius of the PTFE wall at $r = 24$ cm.

3.6.3 A Two-Step Bijective Position Mapping Algorithm

In order to maximize the accuracy of position reconstruction in Run 4, JPM was created as a two-step algorithm which combines field map interpolation with the Delensing technique. The IDW algorithm was chosen as the main interpolation algorithm to work with the field maps since it is simple and efficient on scattered data, and Delensing is subsequently applied to correct out interpolation systematics.

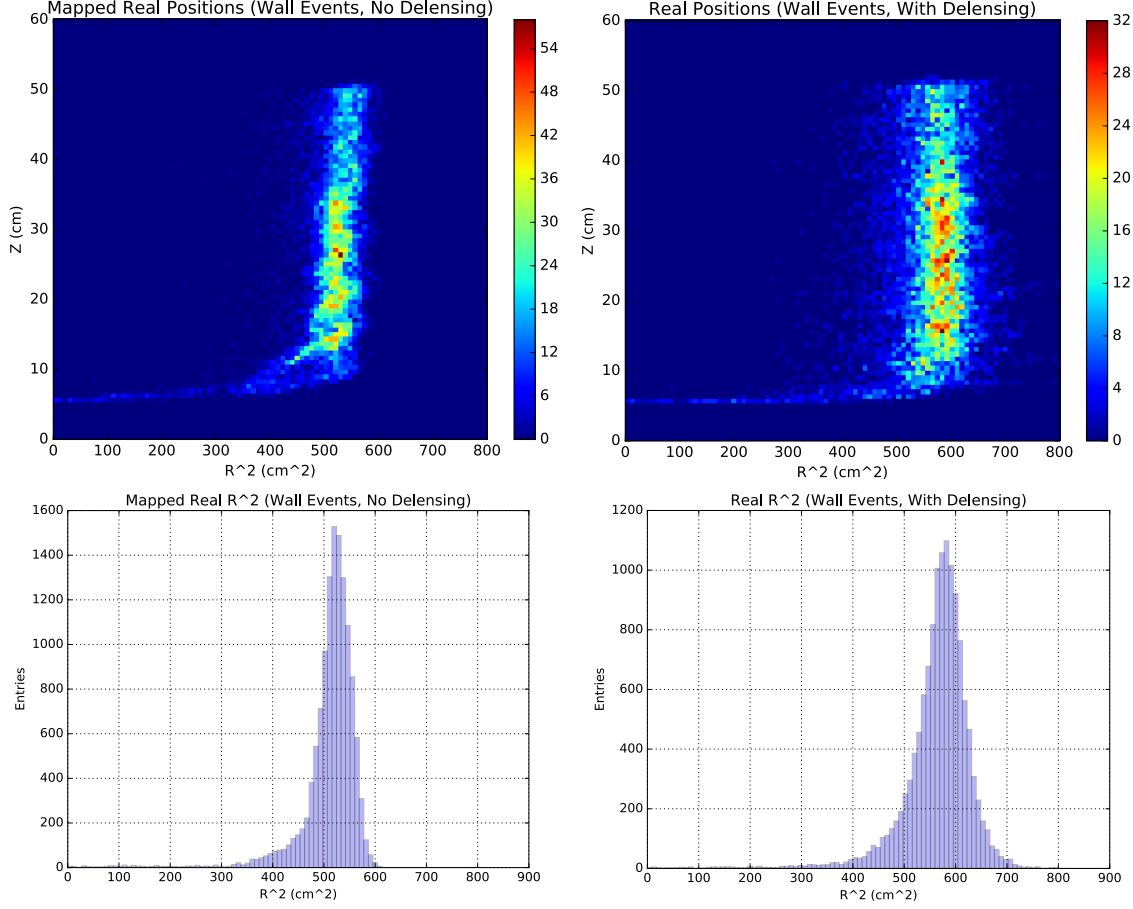


Figure 3.18: (Top left, right) The “rough real space” and Delensed wall data distributions in (r^2, z) space. (Bottom left, right) Projections of the distribution in r^2 , where the wall data mean is clearly shifted to $r \approx 24$ cm.

With flexibility in mind, the algorithm was also designed to be a bijective mapping between S2 space and real space (i.e. the interpolation algorithm works in either domain and Delensing was made to be reversible). While we may want to study fiducialization or background leakage in real space, we may also want to make comparisons with simulations mapped to observable S2 space, making bi-directionality very useful.

The JPM backend and main implementation code are written in C++, but a Python implementation was also built using the Boost-Python library to create a wrapper class. For additional convenience, runtime options allow the user to choose the direction of the mapping (S2 space to real space, or vice versa) as well as turn off the Delensing portion of

the correction if desired.

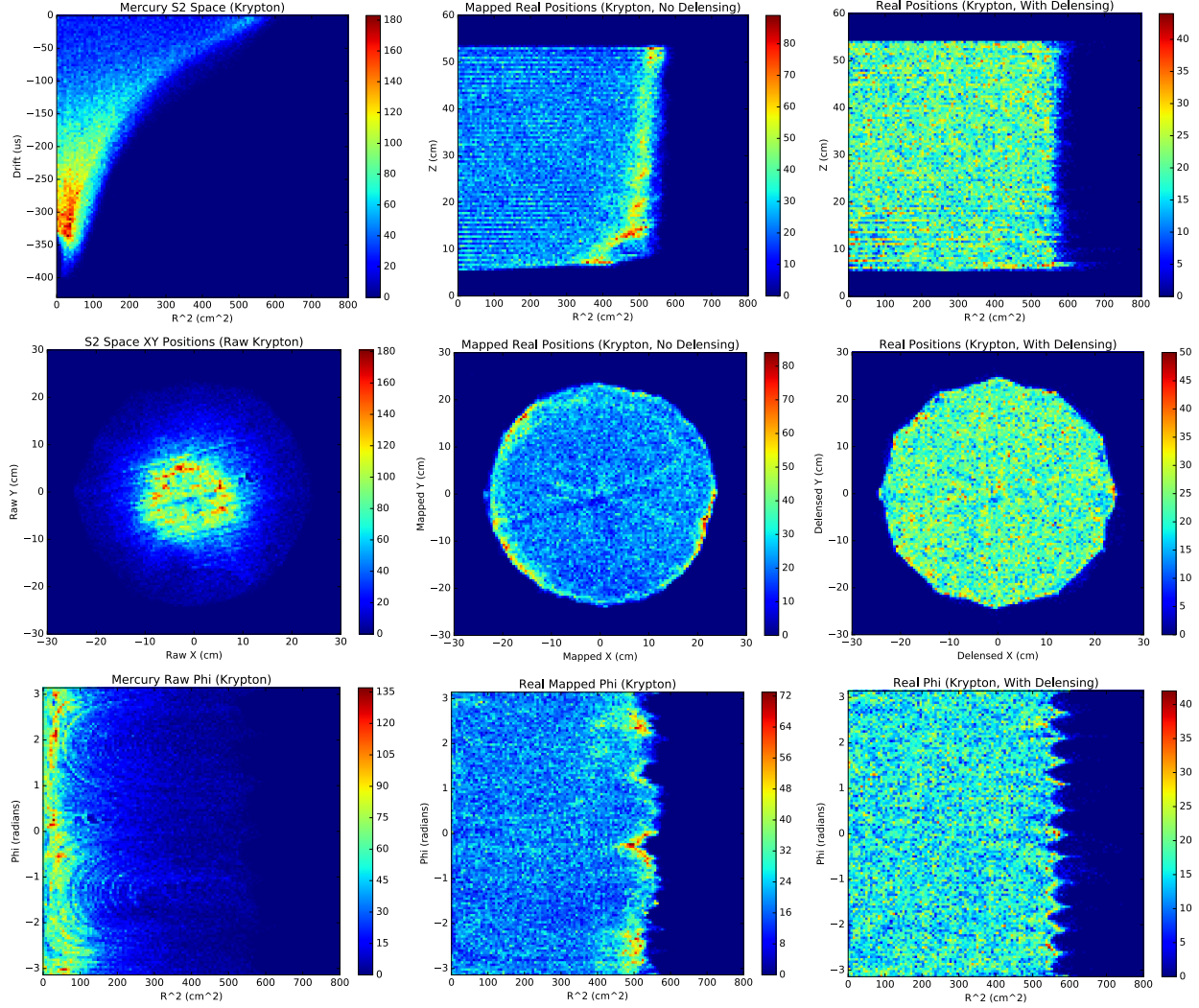


Figure 3.19: (Left) Krypton events in “S2 space” reconstructed coordinates (xy coordinates found by Mercury and drift time). (Middle) Events after IDW interpolation with the field maps (“rough” real space). (Right) Events after Delensing corrections.

To assess JPM’s performance and stability, the full algorithm is tested with each field map and krypton dataset used to generate the correction maps. The result should be a roughly uniform spatial distribution. Results for mapping an example Run 4 krypton dataset from S2 space to real space are shown in Fig. 3.19. The Delensed krypton distributions are indeed very uniform in the bulk, and possess the correct dodecagonal detector shape as enforced in the r^2 correction. There are still “hotspots” at low z and near the walls, but this is not

surprising, since this is where the detector geometry becomes more complex and where the systematic uncertainties are largest.

The error in the full JPM algorithm is exceedingly difficult to quantify, since errors propagate through many algorithms. The field maps themselves have intrinsic systematics associated with the COMSOL model’s discrete charge distribution and simulation inefficiencies (i.e. loss of electrons), the IDW interpolation has associated systematics (particularly in the field-entangled distance metric), and the Delensing algorithm has errors dominated by the krypton bin statistics.

The precision of Delensing is limited by the coarseness of the binning. An adequate number of krypton events is needed in each spatial cell on a per-month basis, and krypton calibration data is finite. One can see the smearing effect due to limited resolution; in the middle left plot of Fig. 3.19 the uncorrected xy distribution shows (despite field effects) a realistic diagonal grid wire pattern from lower-left to upper-right, which is washed out in both mapped distributions.

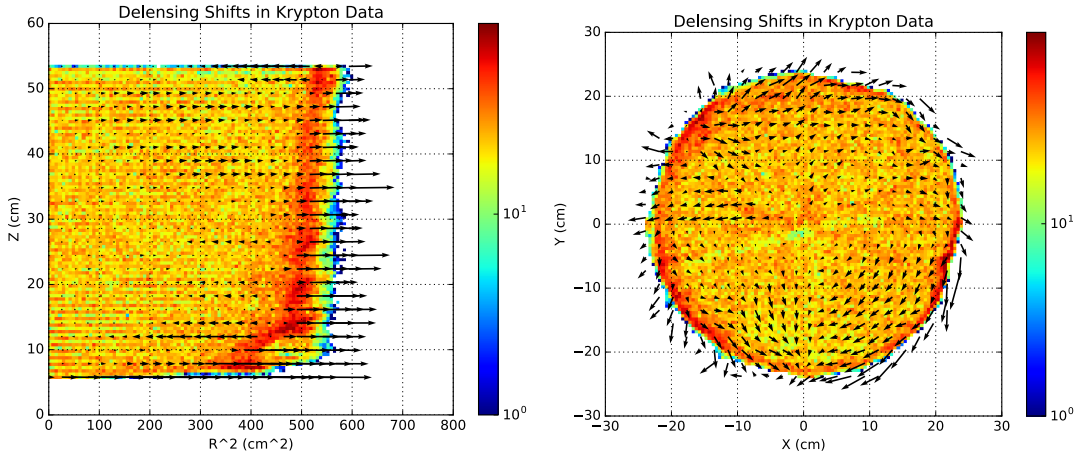


Figure 3.20: Arrow plots showing the displacement of events due to Delensing.

To ensure that the Delensing algorithm is displacing events by physically sensible amounts, we can use “arrow plots” as another cross-check of the algorithm (Fig. 3.20). The average directionality and magnitude of displacement are reasonable based on the over-densities. It should also be noted that high-density regions at the wall generally result in events being

pushed away from the bulk, rather than being pulled into the fiducial region.

JPM was designed as a bi-directional mapping. In the “forward” case, IDW interpolation and Delensing are performed to map from S2 space to real space coordinates; in the “reverse” case, real space coordinates are reverse-Delensed and then interpolated with the real coordinates of field map points (using a normal Euclidean distance metric) to get S2 space coordinates. To test the reversibility of the algorithm, krypton data is mapped from S2 space to real space, then returned to S2 space. The event-by-event residuals are then calculated to quantify the error associated with the reverse mapping (see Fig. 3.21).

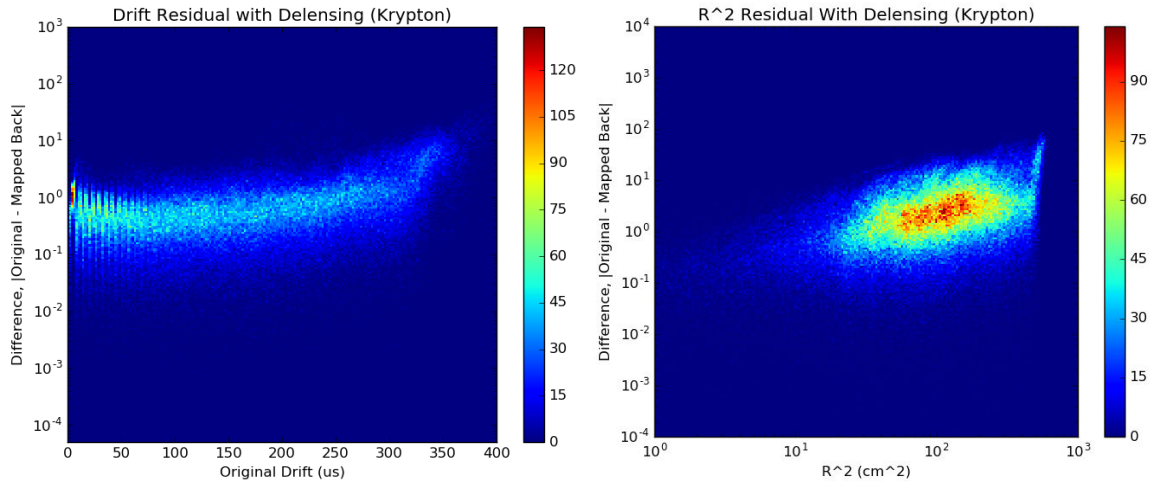


Figure 3.21: Drift time and r^2 residuals as a function of the original S2 space coordinate.

Given the uncertainties in the interpolation, the residuals are impressively small. The majority of events have drift time residuals $\lesssim 2 \mu\text{s}$ and r^2 residuals $\lesssim 10 \text{ cm}^2$. Events with high residuals are concentrated at large drift times and high radius, where there are larger uncertainties. The residuals are identical when Delensing is not used, implying that the Delensing correction is completely reversible and that the reverse mapping error comes almost exclusively from the field map interpolation.

3.6.4 Impact on the Run 4 Analysis

JPM has served as an important tool for the Run 4 WIMP search in many respects:

- It informed fiducialization, particularly with regards to deciding on a coordinate space for the final WIMP search and optimizing the fiducial mass of exposure segments.
- Electric field values can be easily extracted at arbitrary locations in the detector, allowing the calculation of expected signal yields for events.
- The leakage of backgrounds into the fiducial region, particularly from peripheral detector materials, may be assessed by mapping simulations to S2 space observables.
- Ongoing analysis efforts for LUX, such as background and detector performance characterizations, rely on mapping events to real space coordinates.

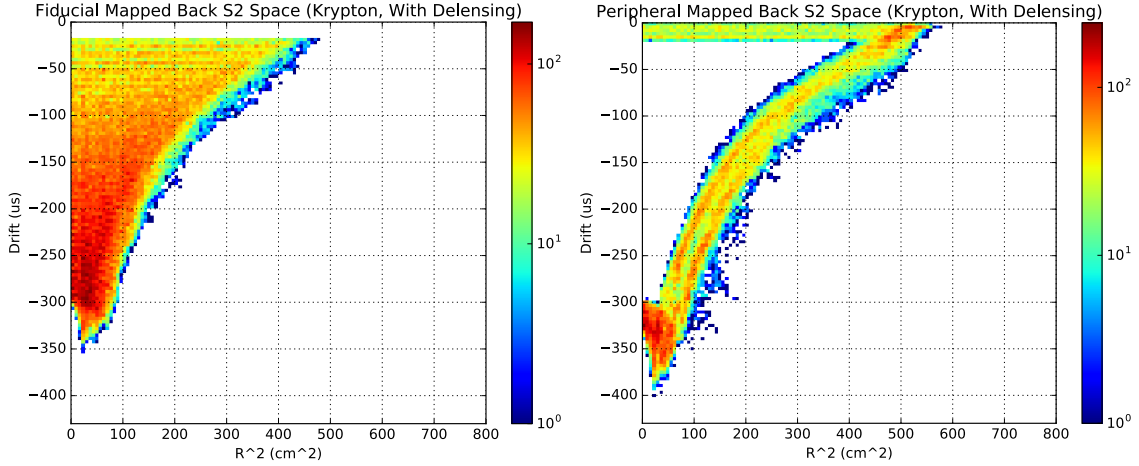


Figure 3.22: (Left) A fiducial selection of krypton events in real space coordinates mapped into S2 space using JPM. (Right) The remaining non-fiducial events mapped to S2 space.

For a WIMP search, it is crucial to understand the fiducial volume and to what extent the systematics affect our DM sensitivity. Shown in Fig. 3.22 is a krypton dataset split into a 22-cm radius fiducial volume and the corresponding peripheral volume, each mapped from real space to S2 space using JPM. The algorithm successfully maps non-fiducial events with minimal scatter into the dark matter search region, and similarly avoids scattering fiducial events into the periphery. Given that DM sensitivity scales as the mass of the target, and the fiducial mass of Xe in LUX scales as r^2 , having tools which help us expand the fiducial

radius without increasing systematic uncertainties is key to higher discovery potential (or, alternatively, a better DM limit).

Chapter 4

Modeling Xenon Response with NEST v2.0

A necessary component for any experiment is simulation. Experimentalists working with noble element detectors often need to estimate or predict their detector response, especially in the planning stages of a project. It is important to develop not only dark matter signal models, but also background models.

The Noble Element Simulation Technique, or NEST, is a software package developed to generate realistic simulations of noble element response to energy depositions. In particular, it began as a precise modeling of S1 and S2 signals in dual-phase xenon TPCs, however it has become (in version 2.0, its second iteration) a more general standalone physics calculator for use with noble element detectors.

The previous iteration NEST v1 was a C++ code directly integrated into the GEANT4 simulation package for modeling detector response. In this implementation, primary particles deposit energy at an interaction site, and the scintillation and ionization yields are calculated using semi-empirical models, whose functional form is based on theoretical first principles and whose parameters are found by global fits to noble element datasets [143, 223]. The resulting photons and electrons are then propagated within GEANT4. In this way, the NEST functions can intervene in the tracking of these secondary particles, and use information

about the electrons reaching the liquid surface to generate realistic S2 signals in the gas phase.

Though successful, this implementation required GEANT4 functionality and used an unwieldy set of hard-coded models and parameters. NEST v2 was thus developed as a standalone C++ software package, with optional linking to GEANT4 and ROOT software for convenience. This new package contains simpler, compartmentalized yield models which are factorized into different interaction types for easier development. The code also performs simplified detector response modeling outside the GEANT4 framework, through user-definable parameterizations of the light collection and electric field profiles. The user may modify various detector parameters and analysis settings via external configuration files.

The improved light and charge yield models for xenon are now completely empirical. This paradigm shift was made necessary by the precision of new experimental results, which over-constrained the old first-principles models. In this chapter, the NEST v2 models and algorithms will be described in detail. In particular, we will present the current Xe response model for heavy ions, including recoil nuclei from nuclear decay.

4.1 Theoretical Underpinnings of Xenon Microphysics

4.1.1 Energy Partitioning in Xenon

While there are many types of particle interactions in Xe, we generally discuss elastic scatters which are classified as either *electron recoils* or *nuclear recoils*, where the particle scatters off an atomic electron or a Xe nucleus (respectively). Energy deposited in these interactions is distributed according to the pathway shown in Fig. 4.1.

There are 3 channels by which energy is deposited in xenon: atomic excitation (production of excitons), ionization (production of ions), and heat through atomic motion (production of phonons). However, these channels are not independent.

Particles recoiling through xenon collide with neighboring atoms, producing heat through the atomic motion. For electron recoils, this energy loss is actually negligible [83, 143, 223];

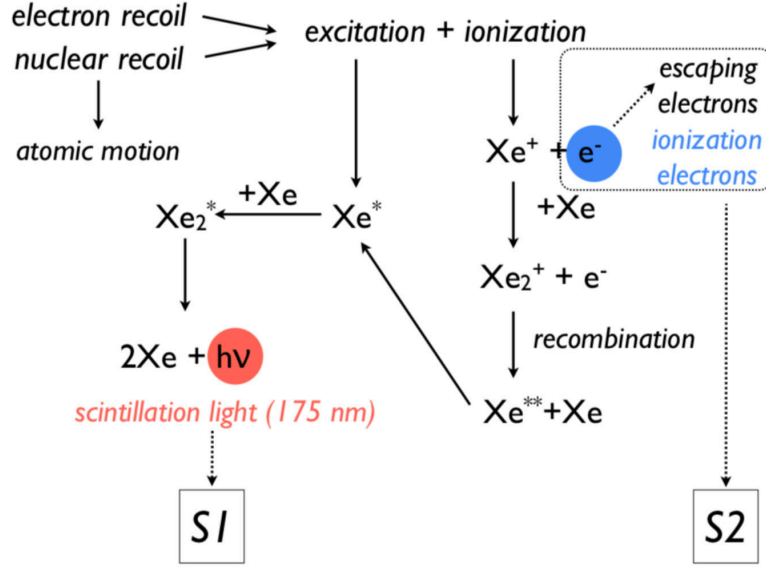


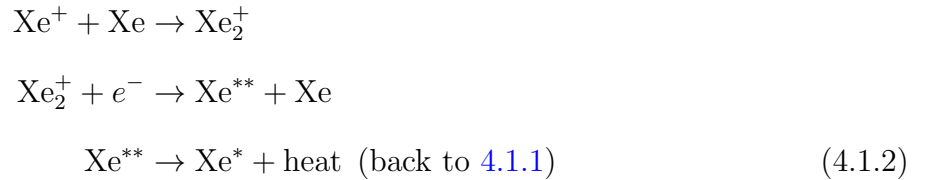
Figure 4.1: A diagram of energy deposition pathways in LXe [202].

for nuclear recoils, this component is significant. In dual-phase xenon TPCs, this heat is not detectable, so there is an overall quenching of the observable quanta for nuclear recoils.

Energy also goes into the formation of excited dimers (excimers) Xe_2^* , which then de-excite to produce 175 nm VUV scintillation photons:



There is also ionization along the recoil track. The electrons produced may either escape (due to diffusion or drift) or recombine with an ionized Xe atom. If recombination occurs, an excited Xe atom is produced, which then feeds back into the production of an excimer and further scintillation:



There are proposed mechanisms which may result in additional quenching of the observed quantum yields. One process comes from Hitachi [39, 124], which involves the collision of

two excitons to produce a low-energy electron:



This “bi-excitonic quenching” leads to an overall reduction in the scintillation yield, since two excitons are consumed in a process which leads to an excimer and thus a single photon.

Penning effects may also play a role in the overall quantum yields, whereby excimers collide to produce a ground state, a molecular ion, and an ionization electron [76, 158]:



This Penning ionization process effectively deactivates an excimer through the ejection of an electron. Furthermore, we can see from Eq. 4.1.2 that these products result in an additional recombination photon as well as undetectable heat loss. Given that two excimers began the process, this reaction results in a net suppression of quanta.

A helpful survey of the many excimer formation and decay processes in Xe is given in [153]. Estimates of the frequency of the various de-excitation mechanisms are provided therein, however it is still unclear to what extent each affects the Xe response.

4.1.2 Recombination Physics and the Combined Energy Scale

It is clear from the available excimer pathways that the two detectable channels are anti-correlated, since the recombination of ions suppresses the number of electrons N_e (S2) and directly enhances the number of photons N_{ph} (S1). However, the statistical recombination process results in wide recombination fluctuations; these fluctuations dominate the energy resolution in either S1 or S2 space.

Rather than reconstructing the energy from scintillation or ionization alone, we can leverage the fact that recombination fluctuations result in the same number of total quanta. The “combined energy scale” E_c is reconstructed from the total quanta as follows:

$$\begin{aligned} E_c &= W N_q = W(N_{ph} + N_e) \\ &= W \left(\frac{\langle S1 \rangle}{g_1} + \frac{\langle S2 \rangle}{g_2} \right) \end{aligned} \quad (4.1.5)$$

where W is the work function to produce a single quantum (well-constrained to be 13.7 eV [83, 143]) and N_q is the total quanta. It should be noted that this equation applies to electron recoils only, since the total quanta are quenched for nuclear recoils by an additional Lindhard factor (this will be discussed in 4.1.3).

As discussed in 3.1, g_1 and g_2 are detector response parameters which map observed S1 and S2 signals to light and charge yields. Rewriting Eq. 4.1.5 in terms of variables $x = \langle S1 \rangle$ and $y = \langle S2 \rangle$ gives

$$\begin{aligned} \frac{E}{W} &= \frac{\langle S1 \rangle}{g_1} + \frac{\langle S2 \rangle}{g_2} \\ \Rightarrow y &= \frac{g_2 E}{W} - \frac{g_2}{g_1} x \end{aligned}$$

Thus, fitting a line in this space allows us to extract the g_1 and g_2 parameters from the slope m and y -intercept b :

$$g_1 = -\frac{bW}{mE}, \quad g_2 = \frac{bW}{E}$$

Taking a linear combination of S1 and S2 using these parameters allows us to plot the combined energy distribution. This effectively projects the S1 and S2 signals along a rotated axis, greatly improving the energy resolution by removing the energy-dependent recombination fluctuations [54, 147] (see Fig. 4.2). This method for energy calibration is known as the ‘‘Doke method’’ [88, 224], and was used in LUX as shown in Fig. 3.4.

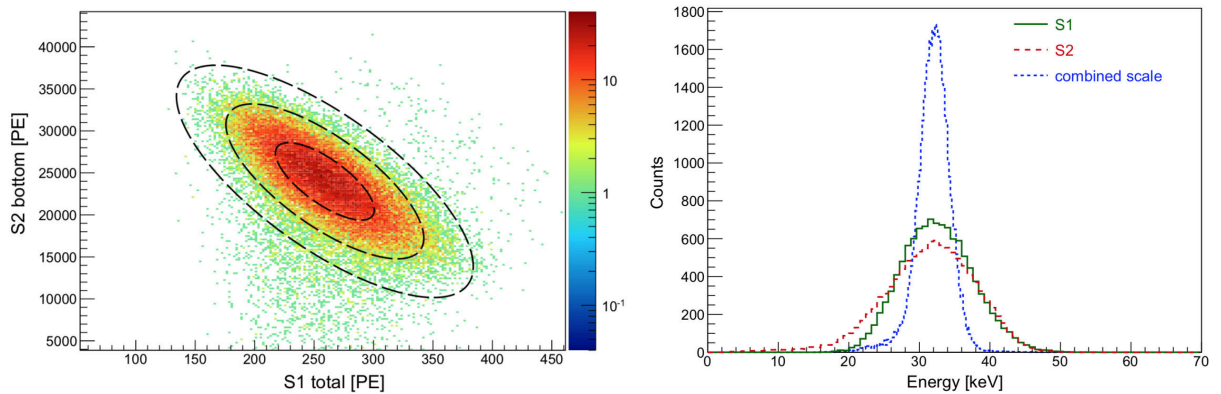


Figure 4.2: (Left) S1–S2 distribution for a population of 32.1 keV krypton events in the Xurich II detector [54]. (Right) S1, S2, and combined reconstructed energies for this line.

The recombination fluctuations have until recently been modeled using a binomial distribution, however the observed variance and dependence of the fluctuations has been shown to disagree with data even after removing known instrumental effects. NEST v2 implements a field- and energy-dependent model for non-binomial recombination fluctuations, with width modifications informed by fits to calibration data from the LUX experiment [22]. The total width of recombination is given by

$$\sigma_T^2 = (1 - p) N_i p + \sigma_r^2$$

where $p \equiv 1 - r$ is the electron escape probability and r is the recombination probability calculated from the exciton-ion ratio as described in [83, 223].

The first term is the binomial variance, which dominates in the limit of isolated electron-ion pairs. The second term is added to empirically broaden the distribution, and dominates for large N_i and therefore high energies; this term is parameterized by ω , and given by

$$\sigma_r^2 \approx \omega p N_i^2$$

for large N_i . The ω parameter is empirically found using available Xe data. This model is found to work well (within errors) for both electron and nuclear recoils.

4.1.3 Lindhard's Theory for Nuclear Recoils

Platzman's equation for rare gases (a modified form of Eq. 4.1.5) expresses the conservation of energy in Xe, through the use of a quenching factor L which takes into the account the energy which is lost to heat in nuclear recoils [143]:

$$E = \frac{N_{ex} E_{ex} + N_i (E_i + E_e)}{L} \approx \frac{(N_{ex} + N_i) W}{L} \quad (4.1.6)$$

E_{ex} and E_i are the energies to create a single exciton or ion respectively and E_e is the average energy of electrons that do not recombine. We assume here that $E_{ex} \approx E_i + E_e$ and that E_e is very small.

This quenching factor L was given in a 1963 theoretical paper by Lindhard, in which he derives an integral equation describing the electronic energy loss in a nuclear recoil cascade

for an arbitrary medium [148]. Lindhard combines the elastic nuclear scattering cross-section, approximated using the Thomas-Fermi model, with the electronic stopping power for low-velocity ions to numerically solve for the initial recoil energy going into electronic excitation.

For the case of $Z_1 = Z_2$ and $A_1 = A_2$ (i.e. the recoiling nucleus is the same species as the medium), this “Lindhard factor” is given by [217]

$$L = \frac{k g(\epsilon)}{1 + k g(\epsilon)} \quad (4.1.7)$$

where k is a proportionality constant between the electronic stopping power and the velocity of the recoiling nucleus,

$$k = 0.133 Z^{2/3} A^{-1/2}$$

ϵ is the energy deposited converted to a dimensionless quantity,

$$\epsilon = \frac{0.8853 a_0 Z^{-1/3} m_2}{Z_1 Z_2 e^2 (m_1 + m_2)} = \frac{0.443 a_0}{m e^2 Z^{7/3}} \quad (4.1.8)$$

and $g(\epsilon)$, which is proportional to S_e/S_n (the ratio of the electronic and nuclear stopping powers), is given by

$$g(\epsilon) = 3\epsilon^{0.15} + 0.7\epsilon^{0.6} + \epsilon \quad (4.1.9)$$

For the case where $Z_1 \neq Z_2$ and $A_1 \neq A_2$, see Sec. 4.4.

It is worth noting that while Lindhard’s model has been shown to work well with solids such as semiconductors, it may be limited in its application to LXe, since there are underlying complexities in the microphysics introduced by recombination [83].

4.2 An Empirical Pathway for NEST v2

In the first incarnation of NEST, global fits to light and charge yield measurements were done to set the 9 free parameters of the original model: 3 for the field and energy dependence of N_{ex}/N_i , 2 for the electric field dependence of recombination, 2 for Penning effects, 1 for the Lindhard k factor, and a nuisance parameter F_0 for continuity at zero-field [143].

In NEST v2, such a complicated fit is avoided. Rather, simple sigmoidal functions with both field and energy dependence are fit directly to light and charge yield data for various

interaction types independently (e.g. β , γ , NR, α , etc.). The mean light and charge yields (and therefore the total number of quanta) are pre-determined models that are integrated modularly into a calculator.

The NEST calculation flow for most models is shown in Fig. 4.3, where the deposited energy E , applied electric field F , and interaction type are inputs to the model, and N'_{ph} and N'_e are the number of photons and electrons output after applied recombination fluctuations. Having a different model for each interaction type is an important feature of NEST v2, since it allows us to modify the calculation flow for a given interaction based on which parts of the model are the most well-constrained by data.

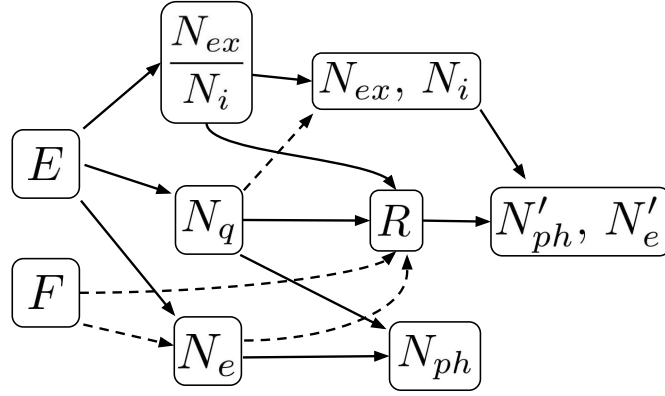


Figure 4.3: The NEST v2 calculator flow for the β , γ , and Xe NR models.

The yields are calculated as follows for β , γ , and NR models:

1. Determine the total quanta N_q from deposited energy E . For nuclear recoils, the Lindhard factor is also applied to quench the number of quanta.
2. Calculate the field- and energy-dependent charge yield $Q_y = N_e/E$, which gives N_e .
3. Obtain N_{ph} using the constraint $N_q = N_{ph} + N_e$.
4. Calculate the energy-dependent exciton-to-ion ratio N_{ex}/N_i and thus N_{ex} , N_i from N_q .
5. Use the field-dependent recombination probability R , which may be obtained from N_{ex}/N_i , to apply recombination fluctuations to N_{ph} and N_e .

The above calculation flow differs for special models. For example, the well-known ER calibration source ^{83m}Kr undergoes a unique scintillation mechanism that necessitates the calculation of N_{ph} prior to N_e . Special nuclear recoils, such as α particles and heavy ions, will be discussed in Sec 4.4.

4.3 ER and NR Model Validations

The ER model in NEST v2 is actually composed of multiple separate models whose usage depends on the interaction type. There are β and γ models, as well as special models formulated for unique sources such as ^{83m}Kr .

The γ model is used for γ interactions of higher energy, including Compton scatters, while the β model is used for both incident electrons (as from a tritium source) as well as low-energy X-rays. We have discovered that for some low-energy applications, a weighted combination of the β and γ models is needed to accurately reproduce data. This may be because the local microphysics of low-energy photon interactions resembles that of recoiling electrons.

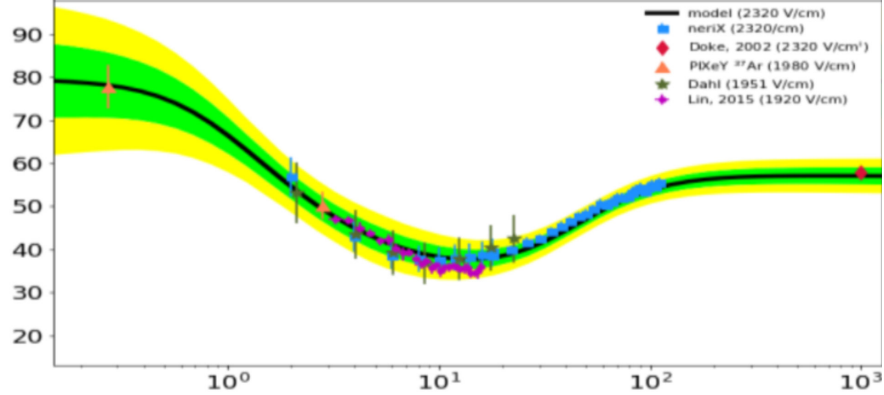


Figure 4.4: ER charge yield model (electrons/keV) at 2320 V/cm compared to data as a function of energy (keV). Green and yellow bands correspond to 1- and 2- σ , respectively [137].

Since there are a variety of ER interactions, we will not go through each model in detail. Given the number of available datasets at various fields and energies, it is also difficult to

succinctly summarize validation results. In Fig. 4.4 we give a comparison of the β charge yield model with some high-field datasets. There is clearly excellent agreement at all energies.

The nuclear recoil model is given by a power law for the total quanta and a set of sigmoids for the light and charge yields:

$$N_q = \alpha E^\beta$$

$$N_e = \frac{E}{\text{TIB} \sqrt{E + \varepsilon}} \left(1 - \frac{1}{1 + (E/\zeta)^\eta} \right)$$

$$N_{ph} = (N_q - N_e) \left(1 - \frac{1}{1 + (E/\theta)^\iota} \right)$$

where α , β , ε , ζ , η , θ , and ι are fit parameters and TIB is the field-dependent “Thomas-Imel box” parameter that determines recombination [155, 165, 217]. This is parametrized as

$$\text{TIB} = \gamma F^\delta \left(\frac{\rho}{\rho_0} \right)^{0.3}$$

where γ and δ are additional fit parameters, F is electric field, and ρ is density with reference density $\rho_0 = 2.9 \text{ g/cm}^3$. For the NR model, anti-correlation is not strictly enforced at low energies, where the number of quanta may fluctuate below zero.

We compare in Fig. 4.5 just some of the world’s NR data with the NEST v2 charge yield model. The NEST model represents data well (within error bars), showing agreement with the latest precision low-energy charge yield data [142]. The most up-to-date benchmark plots for NEST can be found at [168].

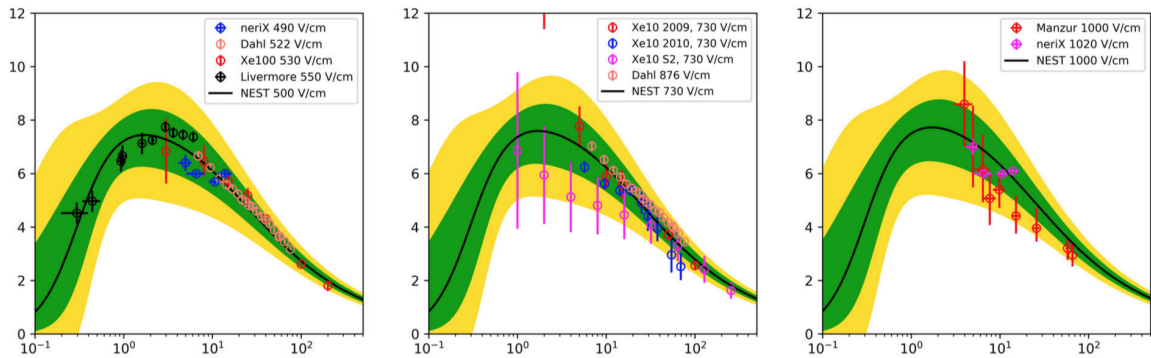


Figure 4.5: NR charge yield model shown with some of the world’s data at various fields [137].

4.4 Developing a Generalized Nuclear Recoil Model

In Sec. 4.1.3, we discussed the case where the recoiling nucleus is the same species as the surrounding medium. However, we would like to develop a model for arbitrary nuclei recoiling through xenon, as from nuclear decay of intruding radioactive isotopes. Here we will examine the case where $Z_1 \neq Z_2$ and $A_1 \neq A_2$ (indices 1 and 2 will hereafter refer to the recoiling nucleus and the species of the medium, respectively).

According to Lindhard theory [148], there is a characteristic energy E_c (E_{1c} and E_{2c} for the two species) at which the nuclear and electronic stopping powers are similar in the medium, i.e. $S_n \sim S_e$. This quantity naturally provides different regimes for approximation; for $E < E_c$ the contribution from nuclear stopping dominates (very little energy goes into electronic motion), and for $E > E_c$ the electronic stopping dominates.

Since most cases of interest to us are within the low-energy regime, we will use the former approximation. Lindhard defines the characteristic energies E_{1c} , E_{2c} , and E_c as

$$\begin{aligned} E_{1c} &\approx \frac{A_1^3 \left(Z_1^{2/3} + Z_2^{2/3} \right)^2}{(A_1 + A_2)^2 Z_1^{1/3}} \cdot (500 \text{ eV}) \\ E_{2c} &\approx \frac{(A_1 + A_2)^2 Z_2}{A_1} \cdot (125 \text{ eV}) \\ E_c &= \gamma E_{2c}, \quad \gamma = \frac{4A_1 A_2}{(A_1 + A_2)^2} \end{aligned}$$

and provides an approximate numerical solution for the sum of energy given to electronic excitation (for $E < E_{1c}$, E_{2c}):

$$\eta = \frac{2}{3} \left(\frac{1}{\sqrt{E_{1c}}} + \frac{1}{2} \sqrt{\frac{\gamma}{E_c}} \right) E^{3/2} \quad (4.4.1)$$

Then, the Lindhard factor, or the fraction of energy lost to electronic excitation, is

$$L(E, A_1, Z_1, A_2, Z_2) = \frac{\eta}{E} = \frac{2}{3} \left(\frac{1}{\sqrt{E_{1c}}} + \frac{1}{2\sqrt{E_{2c}}} \right) \sqrt{E} \quad (4.4.2)$$

This Lindhard factor is used to model the yield of total quantum in NEST. However, we find that the energy dependence of Eq. 4.4.2 leads to insufficient quenching (i.e. too many

predicted quanta) in some cases. It is difficult to estimate where a nucleus becomes too heavy or energetic to use the above Lindhard factor, however we may modify the Lindhard factor with an additional constraint.

The datasets of Doke, Tanaka, and Hitachi et al. for Lindhard quenching of high energy ions (n , α , ^{12}C , Ne, Si, Ar, Fe, ^{206}Pb , and ^{252}Cf) [88, 124, 226] are used to model the atomic mass dependence of the Lindhard factor in the high energy limit. This function then serves as an upper bound on the Lindhard factor used by NEST. The atomic mass dependence of this L_{max} is given by

$$L_{\text{max}}(A) = \frac{a}{1 + (A^2/b)^c} \quad (a = 0.96446, b = 19227, c = 0.99199) \quad (4.4.3)$$

This parametrized fit to data is shown in Fig. 4.6.

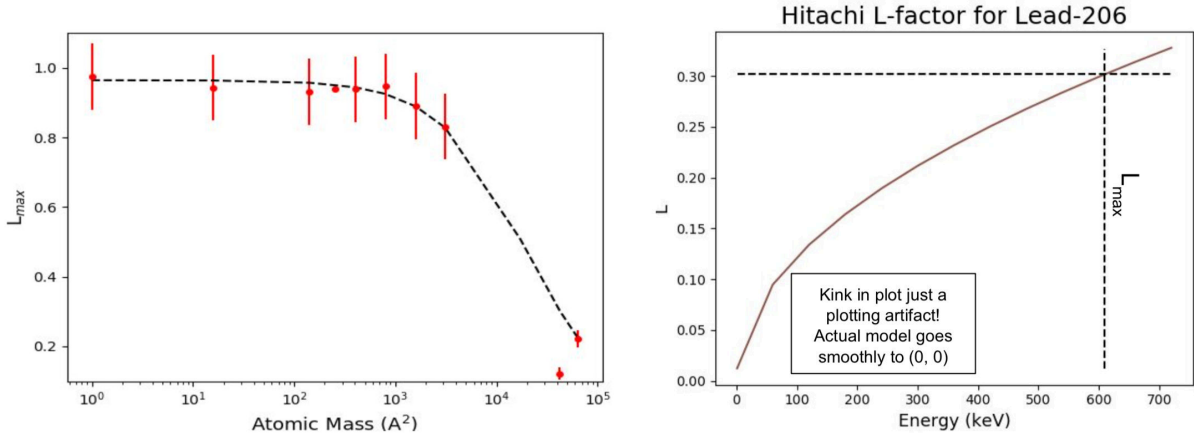


Figure 4.6: (Left) The atomic mass dependence of L_{max} (dotted line) used as an upper bound on the calculated Lindhard factor, along with heavy ion data (red dots). (Right) The energy-dependent Lindhard factor for a ^{206}Pb nucleus (courtesy of Greg Rischbieter of the NEST collaboration).

In the case of α particles, data is more readily available from xenon experiments across a broad range of energies, and thus is treated as a special case. For these nuclei, the empirical Lindhard factor takes the form of a power law in energy:

$$L_{\alpha} = a E^b \quad (a = 0.56136, b = 0.056972) \quad (4.4.4)$$

We would intuitively expect the number of protons in a nucleus to play a role in liberating electrons from Xe nuclei. This motivates the use of an atomic number-dependent power law for the exciton-ion ratio, i.e. the initial partitioning of quanta:

$$\frac{N_{ex}}{N_i} = \alpha + a Z^b, \quad \alpha = \frac{c}{(1 + (\rho/10)^2)^d} \quad (4.4.5)$$

$$(a = 0.00178, b = 1.587, c = 0.64, d = 449.61)$$

where α is a density-dependent parameter which becomes non-negligible for noble elements in the gas phase and ρ is the mass density of the medium.

From the Lindhard factor L and the exciton-ion ratio, it is possible to calculate both the total number of quanta N_q and the number of initial ions created N_i :

$$N_q = \frac{L \cdot E}{W}, \quad N_i = \frac{N_q}{1 + N_{ex}/N_i} \quad (4.4.6)$$

A modified Thomas-Imel box (TIB) model is used to determine the recombination probability for both the α and heavy ion models, which then allows us to calculate the resulting numbers of photons and electrons. The TIB parameter is dependent on mass density, atomic mass, and electric field.

The dependence on field is intuitive, since the electric field pulls electrons from the interaction site and prevents recombination. The dependence of recombination on the drift field F is a power law given by

$$D_F = \begin{cases} \left[1 + \left(\frac{F}{a} \right)^b \right]^c & \text{(Liquid)} \\ \sqrt{F} & \text{(Gas)} \end{cases} \quad (4.4.7)$$

$$(a = 95., b = 8.7, c = 0.0592)$$

The origin of the atomic mass dependence is related to the ionization density in the recoil track. The species of the nucleus determines the stopping power and the resulting track structure, and the sparseness of the track further determines local screening (shielding) of the electric field by the ion cloud. An empirically derived exponential mass dependence term

is found by fitting charge yields from α , ^{206}Pb , and Xe-Xe nuclear recoil data:

$$D_A = a e^{b(A/4-1)} + c \quad (4.4.8)$$

$$(a = 0.02966094, b = 0.17687876, c = 1.0 - 0.02966094)$$

There should be an additional TIB dependence on the density of the medium, since this further influences the track structure. This dependence is an empirical power law:

$$D_\rho = \left(\frac{\rho}{a}\right)^b \quad (a = 0.2679, b = -2.3245) \quad (4.4.9)$$

The resulting TIB parameter then takes the overall form

$$\xi = \frac{a D_A}{D_F (1 + D_\rho)} \quad (a = 0.00625) \quad (4.4.10)$$

which is used to calculate the recombination probability (restricted to be $\in [0, 1]$):

$$R = 1 - \frac{4 \ln(1 + N_i \xi/4)}{N_i \xi} \quad (4.4.11)$$

The resulting number of photons N_{ph} and number of electrons N_e are then

$$N_{ph} = \frac{N_q \cdot N_{ex}/N_i}{1 + N_{ex}/N_i} + R N_i, \quad N_e = N_q - N_{ph} \quad (4.4.12)$$

To validate this heavy ion model, we cross-check the high-energy NEST predictions with the original Doke and Tanaka datasets for various nuclei (see Fig. 4.7). While one dataset is systematically lower than the other, the NEST curve is shown to roughly split the difference. Within the quoted errors, the NEST model matches data well; this is due to the implementation of the $L_{\max}$ constraint at high energies (as shown, these datasets include relativistic ions at 422 MeV and above).

We would like to demonstrate the model at all energies, and compare the response of various nuclei. This is non-trivial, as there are dependencies on atomic number, atomic mass, energy, and electric field. Furthermore, real physical isotopes come in different stable configurations, i.e. with different neutron mass fractions.

To maintain the utility of these models, we calculate the light and charge yields for naturally occurring isotopes, taking into account natural abundances by using the average

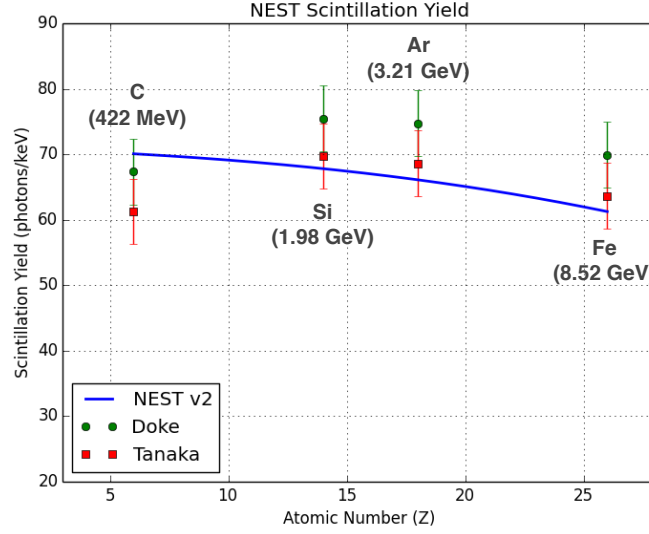


Figure 4.7: NEST model compared with the original Doke and Tanaka data.

atomic mass. In Fig. 4.8, we can see that while there are crossing points of the light yield curves, there is generally a reduction in the light yield as atomic mass increases.

Additionally, there are notable “kinks” in the light yield curve for each isotope, generally at higher energy for larger nuclei, where the light yield becomes very flat. This is due to a moving saturation point, an energy at which the Lindhard reaches its constrained maximum value, resulting in a simple linear energy dependence. The charge yield is much smoother,

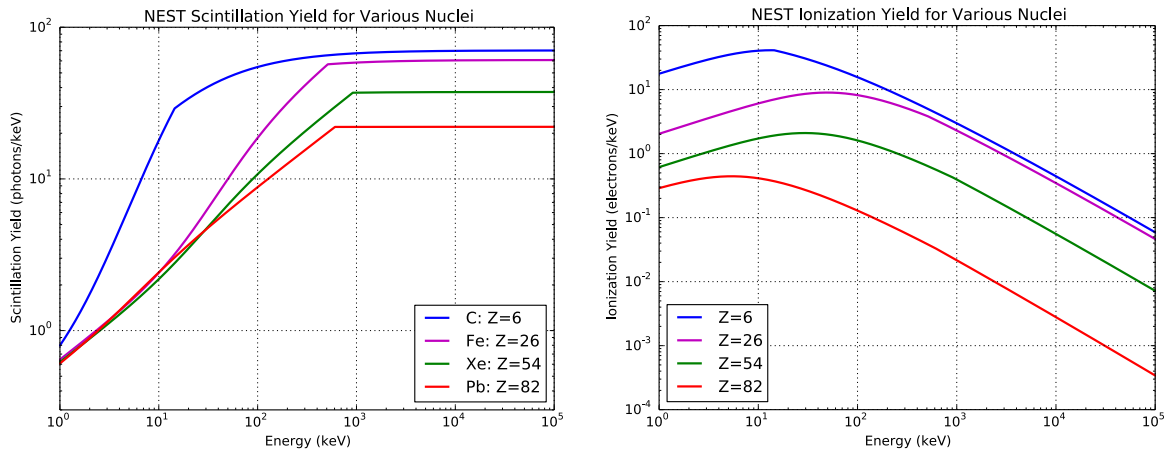


Figure 4.8: (Left) Light yield (photons per keV) for natural isotopes of C, Fe, Xe, and Pb. (Right) Charge yield (electrons per keV) for the same isotopes.

since it is only a small fraction of the total quantum yield, and is less sensitive to sudden changes in the Lindhard factor dependence. Also note that the anti-correlation of light and charge is maintained here, hidden by the axis scales.

We can additionally hold the atomic number constant and study the dependence of the light and charge yields for isotopes resulting from real nuclear decays. As shown in Fig. 4.9, the relationship between atomic mass and the kinetic energy of the nucleus is complicated since it depends on the parent process, however these predictions show the energy dependence of the model.

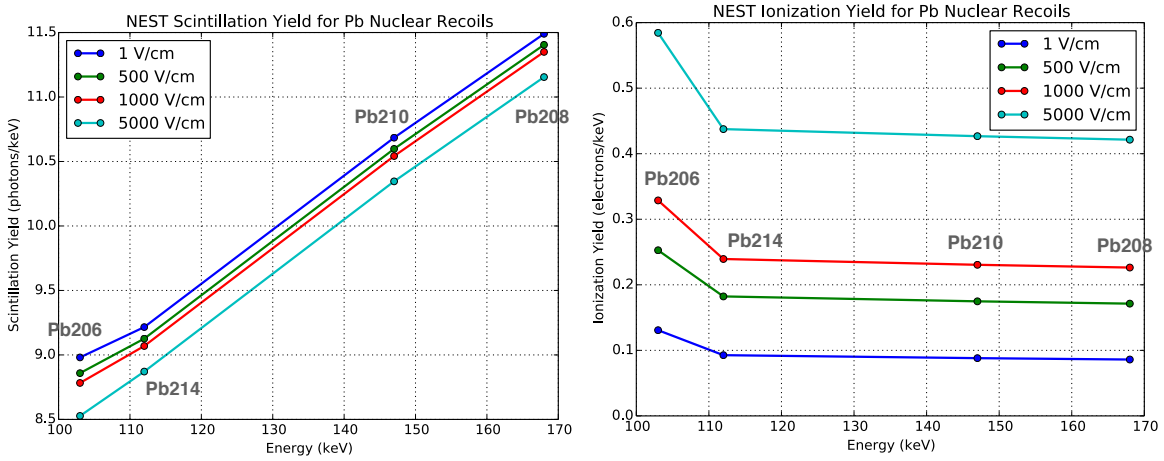


Figure 4.9: (Left) Light yields and (right) charge yields for real Pb isotopes resulting from nuclear decays, for various electric fields.

The field dependence is relatively weak for large nuclei, since the electron fraction is already very small due to the nuclear recoil track structure, field screening effects, and strong recombination. Once again, the plots show the expected anti-correlated behavior.

An important caveat is that these “heavy ion” models do not incorporate any information about the charge distribution for these nuclei. In reality, we would expect for the stopping power and recombination to be affected by the electron cloud of the recoiling nucleus. However, since this model is empirically driven, the employed datasets effectively average over these effects and we are left with charge-independent models. Such effects will be discussed further in Sec. 6.2.

Chapter 5

Implementation of a Triggered Heavy Ion Source in the DAX Detector

The **DA**vis **X**enon testbed (DAX) was developed as a platform for Xe detector R&D at the University of California, Davis. Using the DAX system, we have implemented a dual-phase TPC to perform studies of fundamental xenon physics; collecting data and informing models for Xe response is important for various noble element experiments.

A primary motivation for the construction of the DAX was to carefully study a specific class of nuclear decay backgrounds, namely heavy nuclear recoils from radon progeny, in a dedicated TPC. Multiple methods may be used to employ these backgrounds as deliberate sources for characterization. In this chapter, I will discuss one such method: α -tagging with semiconductor devices. I will demonstrate the development and successful implementation of an α -triggered source of ^{206}Pb using PIN diodes in LXe.

5.1 Motivations for Wall Background Characterization

5.1.1 Alpha Decays

Before delving into nuclear decay backgrounds, some words are in order about the physics of α decays. For this discussion, we will largely follow the treatment given in [\[138\]](#).

It is well known that for atomic nuclei with an atomic mass of ≈ 56 , e.g. iron, the binding energy per nucleon is no longer at a minimum. In fact, the binding energy flattens out and begins to decrease for heavier nuclei, as shown in Fig. 5.1; this binding energy is well-described by a combination of the well-known “liquid drop” and “nuclear shell” models. This means that nuclear disintegration mechanisms (i.e. fission processes) become favored over nuclear fusion, while the ratio of protons to neutrons increases with atomic mass.

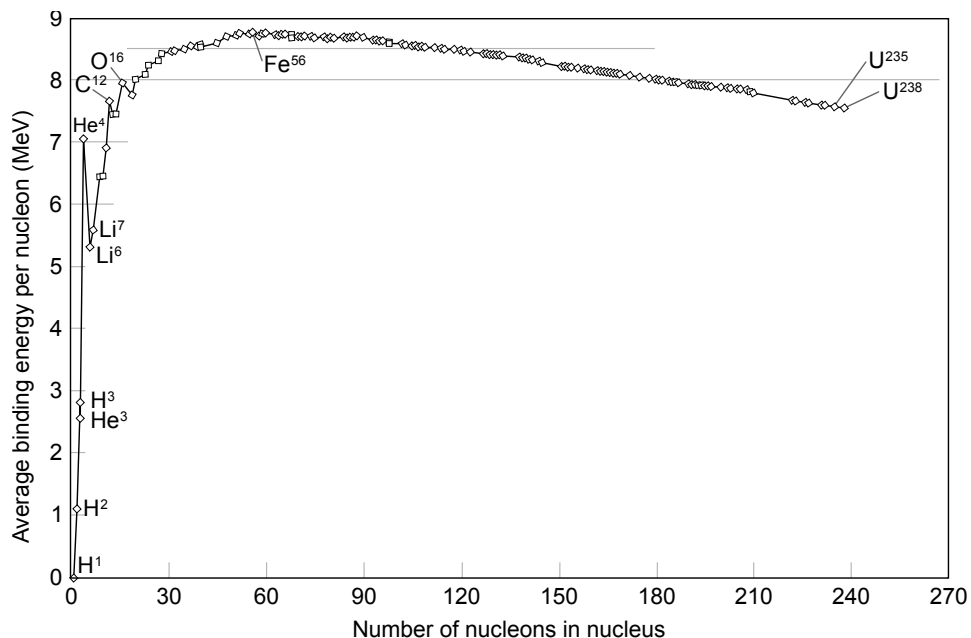


Figure 5.1: Average binding energy per nucleon as a function of atomic mass.

As the atomic mass increases, the size of the nucleus increases as well. However, the Coulomb force increases with size as Z^2 , whereas the nuclear binding force increases more slowly (as $\sim A$). Therefore, it becomes energetically favorable to eject positive charge via a fission process.

Such a spontaneous process involves a release of kinetic energy, which comes from a change to the mass energy of the initial nucleus, $Q = \Delta mc^2$. The particle that is most likely spontaneously emitted is one which has a small mass relative to the mass of its separate constituents, so as to maximize kinetic energy; α particles, or helium nuclei with 2 protons

and 2 neutrons, satisfy this requirement. In fact, for heavy nuclei, an α is one of the only light nuclear structures whose emission results in a net energy release. Through α decay, the nucleus slightly reduces the overall proton to neutron ratio and transitions to a more stable nuclear configuration.

The “ Q -value”, also known as the disintegration energy, is the loss of binding energy that is converted into the summed kinetic energy of the decay products. α decay processes follow

$${}^A_Z X_N \rightarrow {}^{A-4}_{Z-2} Y_{N-2} + \alpha \quad (5.1.1)$$

Using energy conservation with the above equation gives the following Q -value:

$$Q \equiv (m_X - m_Y - m_\alpha)c^2 = T_Y + T_\alpha \quad (5.1.2)$$

where T is kinetic energy, X denotes the parent nucleus, and Y denotes the daughter nucleus.

Since the α is much lighter than our decaying nucleus, it absorbs most of the kinetic energy. We can easily quantify this by assuming non-relativistic velocities here, i.e. $v_\alpha \ll c$. If X is at rest initially,

$$\begin{aligned} |p_Y| &= |p_\alpha| \\ 2m_Y(Q - T_\alpha) &= 2m_\alpha T_\alpha \\ \implies T_\alpha &= \frac{Q}{1 + m_\alpha/m_Y} \end{aligned}$$

Since $m_\alpha = 4$ and $m_Y = A$, we then simplify the above result to

$$T_\alpha = \frac{Q}{1 + 4/A} \approx Q \left(1 - \frac{4}{A}\right) \quad (5.1.3)$$

As expected, $\approx 98\%$ of the Q -value is typically carried off with the α as kinetic energy. The rest goes into the recoil of Y .

5.1.2 The ^{238}U Decay Chain and Radon Plate-Out

There is a set of radioactive series, or nuclear decay chains, that naturally occur from primordial unstable nuclei. Primordial nuclides are species of nuclei that have been present on

earth since the planet was formed; these parent nuclei then undergo subsequent decays (with half-life of order 10^9 years) into chains of daughter nuclei.

There are 3 such naturally occurring primordial chains: the thorium series (starting from ^{232}Th), the uranium series (starting from ^{238}U), and the actinium series (starting from ^{235}U). The ^{238}U decay chain is shown in Fig. 5.2.

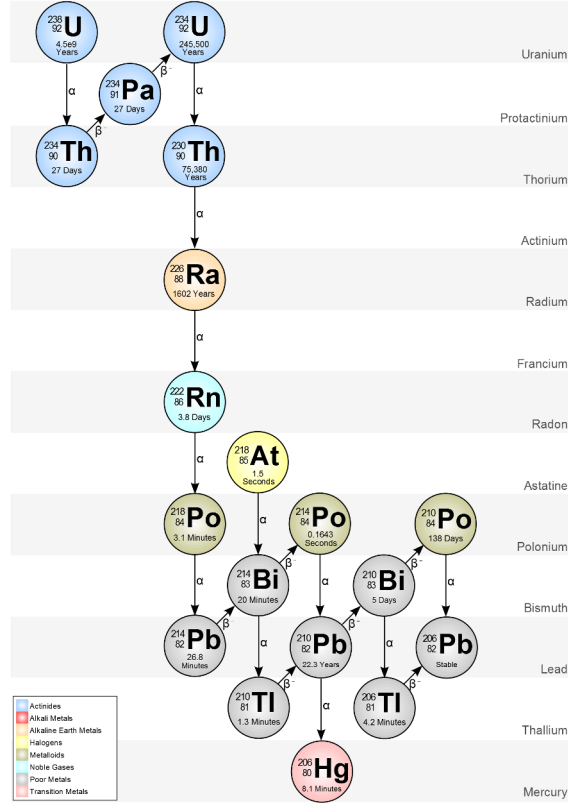


Figure 5.2: The ^{238}U decay chain, courtesy of [169].

It is well-known that ^{222}Rn , a daughter of this decay chain and a noble gas, is emanated from the earth and disperses throughout the air. Thus, any materials exposed to air are also exposed to this radioactive daughter, which may undergo α decay and implant radioactive daughter nuclei into material surfaces. This process is called “radon plate-out” [166, 198]. The radon progeny then continue this implantation process through the decay chain.

This decay chain is therefore highly relevant in rare event searches, such as experiments searching for WIMPs or $0\nu\beta\beta$ decay. The radon progeny embedded in the skin of detector materials is a form of radioactive contamination that increases backgrounds through α or

β decay, where the resulting particles are possibly ejected into the active region of the detector. This is clearly problematic for many experiments [2, 31, 42, 44, 52, 67, 134, 146, 184, 240], and there have been many devoted studies of such backgrounds. Significant efforts have also been made to reduce radon contamination of such experiments through careful material screening, dust minimization through air filtering techniques, and continuous radon monitoring [69, 163, 164].

5.1.3 Heavy Nuclear Recoil Backgrounds

In the LUX experiment (covered in Chapter 3), there have been extensive studies of wall backgrounds resulting from the decay chains discussed above. Moreover, these localized “wall events”, or backgrounds occurring at the boundary of the active Xe, have been used to inform background models and reconstruct the detector wall [67, 141].

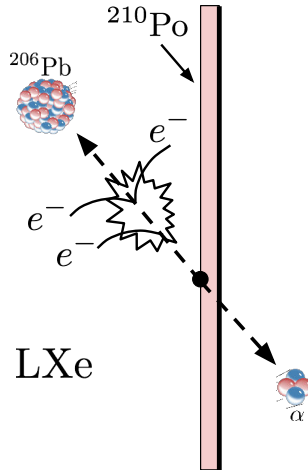


Figure 5.3: An illustration of ^{210}Po decays at the detector wall.

We can assess the rate of these wall backgrounds from the easily distinguishable α spectra, and hope that fiducialization removes any instances of the resultant daughter nuclei penetrating into the active region. However, it is hard to estimate how many of these nuclear recoil backgrounds will be reconstructed in the fiducial volume for a number of reasons:

- Charge loss mechanisms resulting in strong S2 variation at the detector walls.

- Electric field non-uniformities in the periphery.
- Position reconstruction error, which is intrinsically higher near the wall since it is dependent on the S2 signal size.

To make matters more unclear, these variables are highly entangled. For instance, charge loss may result in large variation in the S2 signal near the walls, which increases the position reconstruction error. Electric field non-uniformities may cause yield fluctuations or suppression of detected electrons, also resulting in increased position reconstruction error. Additionally, it may be that electric fields (either radial or azimuthal) are at least partially responsible for charge loss at surfaces, though there may be other factors such as microscopic surface variation [141].

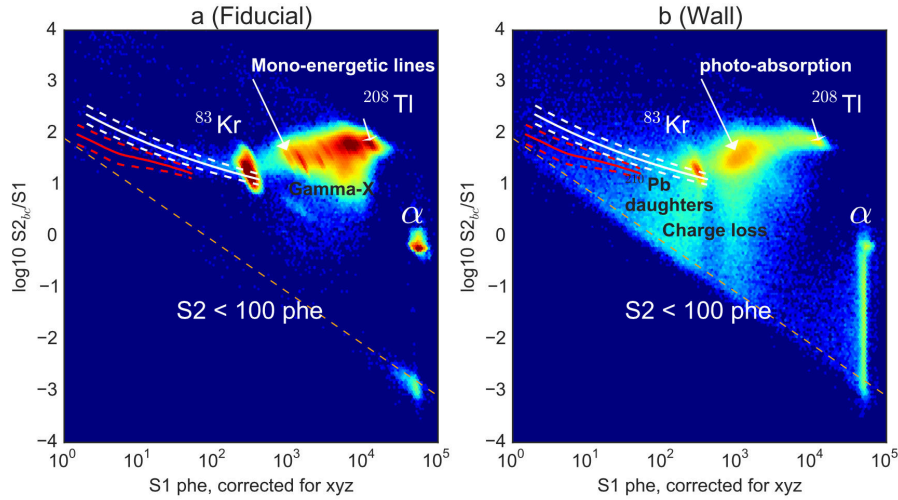


Figure 5.4: (Left) Fiducialized background events from LUX Run 3, with NR band in red. (Right) Run 3 background events near the PTFE walls, as defined in [141]. From [29].

Shown in Fig. 5.4 is an example of the smearing of wall backgrounds due to charge loss. It is clear that tight fiducialization ($r < 15 \text{ cm}$, drift from 10 to $320 \mu\text{s}$) minimizes the bleeding of backgrounds into the NR band, and that there is significant variation in the S2 size across a wide range of energies in the periphery. It is also noteworthy that the α population, which has a very tight S1 distribution, has such enormous variation in its S2

signal; one can see that they have a low charge-to-light ratio to begin with, perhaps implying localized recombination effects.

As mentioned in our discussion of the Run 4 results (see Fig. 3.8), reasonable fiducialization does not guarantee removal of all ^{206}Pb contamination, due to the aforementioned detector effects. This particular background, resulting from ^{210}Po decays, will be our primary focus for the remainder of this thesis.

5.2 Using PIN Diodes to Tag Alpha Decays

As previously mentioned, we would like to employ a method of tagging and monitoring such nuclear recoil backgrounds in Xe detectors. One way of doing so is by implementing an α -tagging detector whose surface is intentionally doped with a source of nuclear recoils such as ^{210}Po . As we will see, PIN diodes serve as excellent α detectors, given the completeness of charge collection and the ability to operate at Xe temperatures.

By immersing such a device in a Xe TPC, we can perform an *in situ* characterization of the Xe response to these ^{206}Pb nuclear recoils. Furthermore, by utilizing such a technology in dark matter searches, it may be possible to compare triggered events with un-triggered wall backgrounds in order to monitor their rate during dark matter searches.

5.2.1 Range of Alphas in Detection Media

Given its relevance to both Xe microphysics and PIN signals from traversing α particles, some words are in order about charged particle interactions in matter.

Fast (i.e. relativistic) charged particles traversing through matter interact with electrons through single collisions, leading to small energy losses of the primary particle with high variance. However, heavy charged particles of intermediate energy are described well by Bethe's theory, which extended the Rutherford free scattering cross-section to interactions in matter by correcting for the electronic binding [225].

As a charged particle such as an α moves through a material, it produces heat, atomic

excitations, ionization electrons; some of these electrons may be so energetic that they produce secondary ionizations known as “ δ -rays” in the neighborhood of the ionization track. The primary particle loses energy to the medium, and this energy lost per unit length is called the stopping power, or specific energy loss. The electronic energy loss component (excitation, ionization) is known as the linear energy transfer (LET).

The average stopping power can be expressed via the Bethe formula, which can be simplified with a non-relativistic approximation [135]:

$$\langle S \rangle = - \left\langle \frac{dE}{dx} \right\rangle = \frac{4\pi Z^2 e^4}{m_0 v^2} n \zeta \left[\ln \left(\frac{2m_0 v^2}{I} \right) - \ln \left(1 - \frac{v^2}{c^2} \right) - \frac{v^2}{c^2} \right] \quad (5.2.1)$$

where the second and third terms may be excluded in the non-relativistic approximation. Here, n and ζ are the number density and atomic number of the absorber atoms respectively, and m_0 and v are the mass and velocity of the incident particle with charge Ze . The quantity I is the mean excitation/ionization potential, which is found empirically for a material. The stopping power is proportional to the number density and size of target atoms, since the probability of interaction increases.

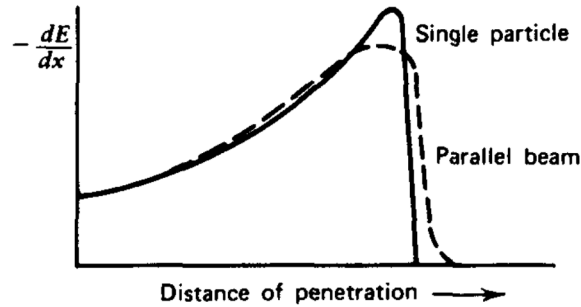


Figure 5.5: An example of a Bragg curve, or stopping power distribution [135].

A plot of the stopping power, Fig. 5.5, shows that particles lose a large portion of their energy near the end of their ionization track. The sharp turnover is called a “Bragg peak”, and indicates the range, or penetration depth. It is possible to estimate the mean range R of incident particles with initial energy E by using the stopping power:

$$R = \int_0^R dx = \int_0^E \frac{dE}{-\langle dE/dx \rangle}$$

One can numerically calculate values for $R(E)$, if the ionization potential is empirically known. However, range measurements also exist from experimental data; the range of α particles in silicon is given in Fig. 5.6. They are relatively heavy charged particles, and thus have a low range. From this figure, we see that a 5 MeV α travels $\approx 25 \mu\text{m}$ in silicon. This roughly determines the minimum thickness of silicon that is needed for a detector to completely stop such a particle and capture the full α energy.

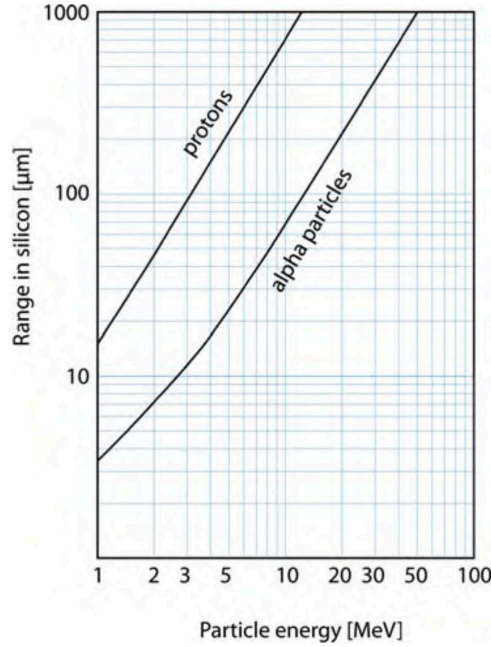


Figure 5.6: The range for alphas and protons in silicon [227].

5.2.2 The Structure of a PIN Diode

A PIN diode is a semiconductor device known as a P-I-N junction, composed of different types of doped silicon. Doping is the mixing of impurities in a controlled concentration into the silicon, resulting in the modification of the material properties.

The introduction of “donor” or “acceptor” atoms into the silicon shifts the corresponding band gap, or the energy needed to transition donor electrons to the conduction band or holes down to the valence band. This means that charge carriers are introduced to the silicon, as

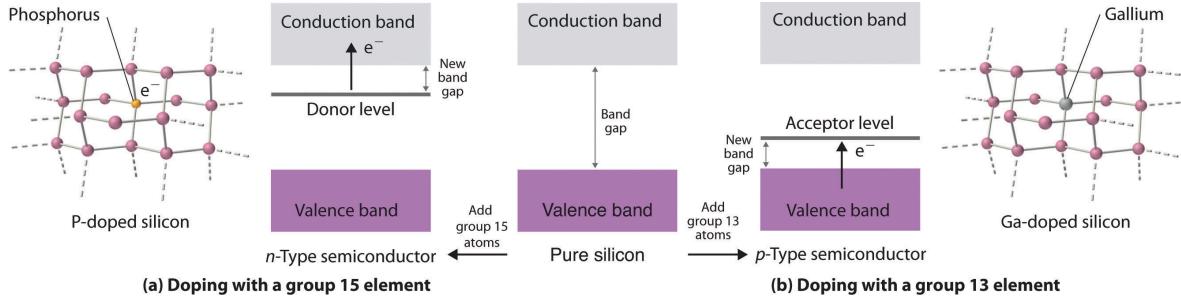


Figure 5.7: Illustration of modified band gaps in doped semiconductors.

conductive holes or electrons. When an intrinsic region, or lightly-doped I-type silicon, is sandwiched between P-type silicon (doped with acceptor atoms) and N-type silicon (doped with donor atoms), a PIN junction is formed.

In such a configuration, the mobile charge carriers tend to diffuse throughout the junction and into the oppositely-doped regions. However, these charge carriers then leave behind oppositely-charged sites which cause a built-in electric field to be formed, which counteracts the diffusion. Once equilibrium has been reached, a stable “depletion region” has been formed in the intrinsic region which is depleted of charge. By biasing this junction with an applied voltage, one can then either vary the resistance with voltage (in forward bias) or increase the size of the depletion region by increasing the field (in reverse bias) [220].

5.2.3 Using a PIN Diode as an α Trigger

By reverse biasing a PIN diode, we create a depletion region which spans nearly the thickness of the chip (the intrinsic region usually makes up the majority of the PIN structure). This then serves as a charge particle detector, since radiation passing through the depletion region produces electron-hole pairs, which are swept to opposite ends of the diode for charge collection. PIN diodes have been used for various detection applications [133, 163, 210].

Using PIN diodes, it is possible to tag α particles capturing the generated charge signals. Furthermore, since α particles of 2.5–10 MeV have corresponding ranges of $\approx 10\text{--}70\ \mu\text{m}$ in silicon (Fig. 5.6), a depletion region thickness of $\sim 100\ \mu\text{m}$ is sufficient for complete energy capture of most α particles.

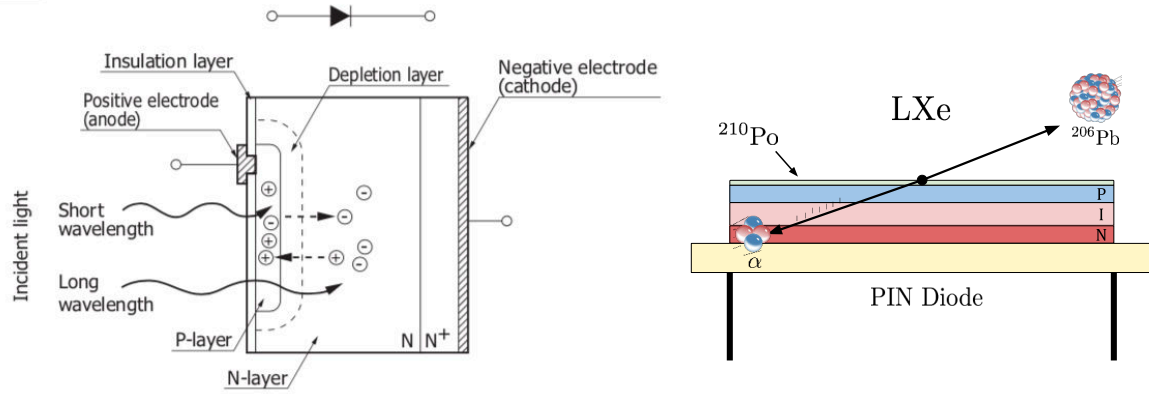


Figure 5.8: (Left) Diagram of a Hamamatsu PIN diode [113]. (Right) An illustration of a ^{210}Po decay on the PIN surface.

This does assume maximum depletion of the PIN and neglects the angular kinematics of the α emission, however such effects can be measured from the collected charge spectrum. Concerns regarding a “dead layer” on the surface of PIN detectors have been addressed for previous experiments [236], but the sub- μm measured dead layer does not significantly affect α -tagging capabilities.

5.3 Creating a Dual-Phase TPC

To demonstrate the viability of such an α -triggered source, we developed a dual-phase Xe TPC for use in the DAX system. Since we wish to localize the source in our Xe TPC using both the light and charge information, the source must be oriented so as to drift charge; however, we also needed to reverse bias the diode to maximize α charge collection. Therefore, the PIN diode was implemented as part of the cathode, with the source facing up into the chamber. A simplified schematic of the TPC layout is shown in Fig. 5.9.

While the PIN diode faces up from the cathode, a Hamamatsu R6041-406 2-inch PMT faces down into the chamber through a PTFE “socket” to detect VUV scintillation photons from the ^{206}Pb nuclei ejected into the LXe. A set of high voltage mesh grids, the gate and anode, are positioned just below and just above the liquid surface respectively, to provide a

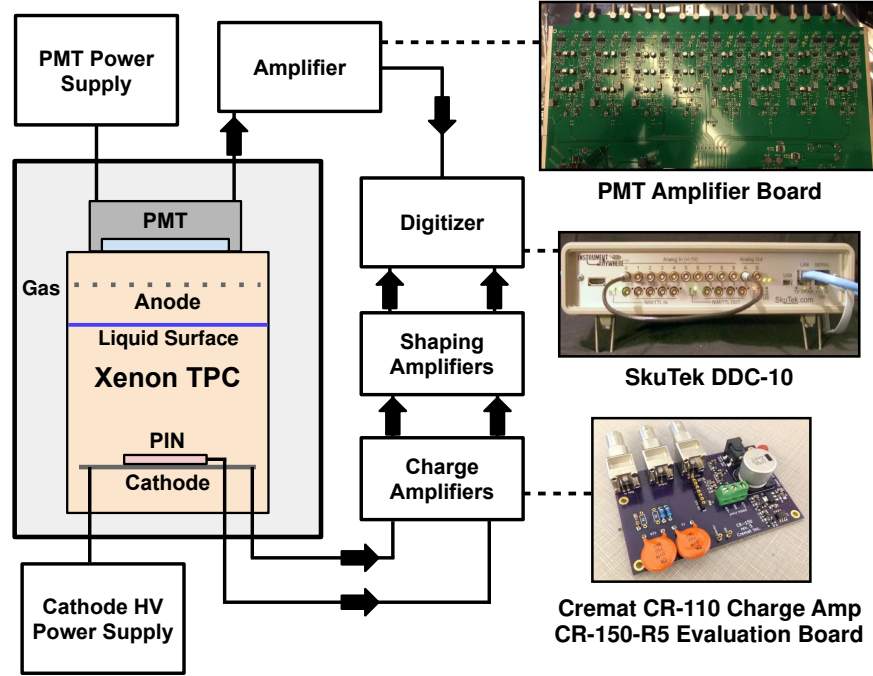


Figure 5.9: A diagram of the DAX Xe TPC setup for PIN-cathode operation.

strong extraction field across the gas gap. The cathode and the gate are set at voltages such that a drift field is produced in the LXe.

The PMT and high voltage electrodes are all independently biased using external power supplies, through low-outgassing PTFE-insulated cables with gold-plated pins which meet SHV feedthroughs at the warm end of the Xe space. The PMT is operated at ≈ 800 V, whereas the HV electrodes are operated at substantially higher voltages. For this iteration of the DAX detector, the anode, gate, and cathode are held at approximately +3, 0, and -1.5 kV respectively.

As we will discuss, a special circuit is used on the cathode for readout of the floating PIN diode. Decoupled charge signals from the PIN diode are fed to a DB9 feedthrough using PTFE-insulated coaxial cables, where they are externally sent through a Cremat CR-110 charge amplifier and a subsequent NIM shaping amplifier module. The PMT signals are fed to a DB25 feedthrough, where they are externally shaped and amplified with a prototype board designed for the LZ experiment which has both low gain and high gain output channels.

Amplified signals from the cathode circuit as well as the PMT are then fed into a SkuTek DDC-10 digitizer for triggered event recording with 10 ns sampling.

As previously discussed, PTFE is a machinable plastic with ideal outgassing and optical properties for Xe TPCs. Thus, the TPC itself is constructed from an assortment of PTFE spacers of various heights which sandwich the high voltage electrodes on a set of PEEK threaded rods. This design allows for easy reconfiguration and assembly of the detector.

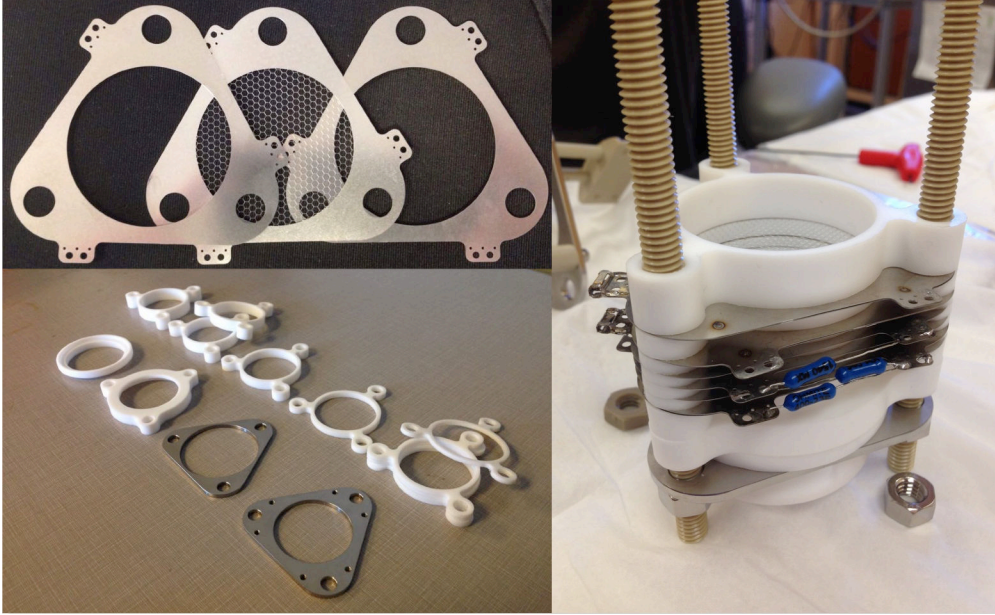


Figure 5.10: (Top left) Grid mesh flanked by FSR pieces. (Bottom left) Separated PTFE spacers and PMT holder components. (Right) TPC partially assembled on PEEK rods.

To ensure uniform drift fields, a set of field-shaping rings (FSRs) are placed at equal intervals between the cathode and gate and connected with $1\text{ G}\Omega$ resistors to evenly step the voltage. The gate and anode grids, as well as the FSRs, were etched from thin stainless steel by Great Lakes Engineering; the gate and anode are $50\text{ }\mu\text{m}$ -thick pieces with a 2 mm center-to-center pitch hexagonal mesh, while the FSRs are $200\text{ }\mu\text{m}$ mesh-less pieces. The hexagonal mesh is chosen to maximize both photon and electron transparency in the extraction region.

In order to achieve dual-phase Xe operations, we must be capable of filling the detector with LXe to the desired level between the gate and anode. Therefore, we developed a simple capacitive level meter consisting of a PEEK mounting plate and stainless steel capacitor

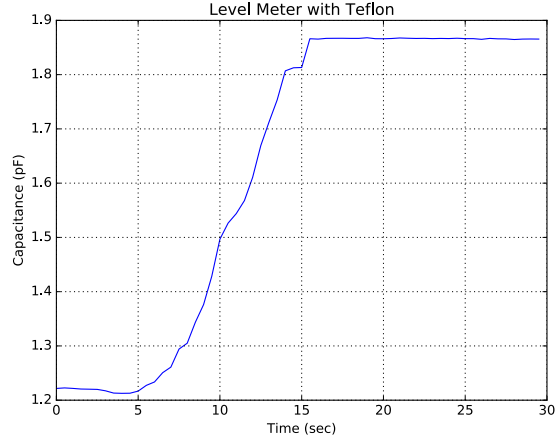


Figure 5.11: (Left) A capacitive level meter to hang alongside the TPC. (Right) A test of the capacitance rise with the insertion of a PTFE card.

plates. The PEEK structure is suspended along the side of the TPC using a set of PEEK rods cut to length, so that the plates are flush with the gate and anode. A pair of coaxial cables (with shields tied together) runs from the plates to a DB9 feedthrough, where they are fed into a Smartec UTI capacitive sensor and USB Toolkit board for serial communication. We use a 2 pF reference capacitor on the UTI board, which is comparable to the designed capacitive range of our level meter. The UTI chip is a sensor-to-time signal converter which cancels stray capacitance to determine the capacitance between the two sensing elements, leading to a direct measurement of the liquid level as the dielectric changes between the plates.

5.4 Development of the ^{206}Pb Triggered Source

5.4.1 Metal Chelation and Surface Adhesion Using TMS-ED3A

Developing a reliable triggered ^{206}Pb source begins by ensuring adhesion of the ^{210}Po to the silicon surface of the PIN diode, so that it is not leached over time into the LXe. In addition to preventing the measurement, this would also create unwanted contamination of the detector space.

We use a dilute acidified solution of n-(trimethoxysilylpropyl)ethylenediaminetriacetate (hereafter called TMS-ED3A, or referred to as an “adhesion promoter”) to covalently bond ^{210}Po ions to the passivated silicon surface of a PIN diode, providing superb adhesion in non-polar aprotic solvents (e.g. xenon).

This chemical is a silane type adhesion promoter, due to the presence of the group called propyl-trimethoxysilane (TMS), which is common in the chemical and polymer industry [92]. Such chemicals adhere well to glass, ceramics, metals, and semiconductors like silicon, and do not adhere as well to plastics, graphite, and noble elements. The TMS group is able to hook onto the the triacetate, so that when it subsequently finds bonding sites on the deposition surface it acts as a “sticking” agent for the whole molecule.

The other major component is the ethylenediaminetriacetate (ED3A) group. ED3A is very similar to ethylenediaminetetraacetate (EDTA), which is a popular chelator for heavy metals in many medical and industrial applications [47, 50, 51, 119]. The molecule works by surrounding a metal ion in solution and forming multiple weak bonds to prevent dissociation. Furthermore, because the molecule has one less acetate than EDTA, it has a bonding site for the TMS group to hold on to. This means the compound serves as both a chelating agent to complex metal ions and an adhesion promoter to bond these complexes to a substrate.

A complication is that the Po^{2+} ion has a high reduction potential, allowing it to steal electrons from the aqueous solution and plate out as a base metal before reacting with our adhesion promoter. A complexing agent is needed to temporarily react with the polonium and prevent this process [99]. Hydrochloric acid (HCl) introduces the necessary Cl^- ion to do this; however, due to the alkaline nature of the adhesion promoter starting solution, an excess of H^+ can create undesirable side reactions whereby the TMS-ED3A bonds to itself and becomes less effective. These competing effects may be balanced with a proper dilution of the HCl solution, facilitating both the chelation and surface bonding of the metal.

5.4.2 ^{210}Po Deposition Procedure

Our deposition procedure is fixed by our low target rate for the polonium source (5 Bq). To begin with, 1 mL of diluted HCl (JT Baker MEMS grade diluted with DI water to 0.01% by weight) was added to our polonium vial (Spectrum Techniques 3700 Bq liquid source, 25 μl , 3% HCl by weight). The HCl acts as both a solvent to extract the polonium from the vial and as a complexing agent during deposition. Two droplets ($\approx 1/8$ mL) of the HCl-Po mixture is transferred to 11.2 mL of DI water, diluting it further by a factor of 90. Two drops of the resulting solution then contains ≈ 5 Bq of ^{210}Po .

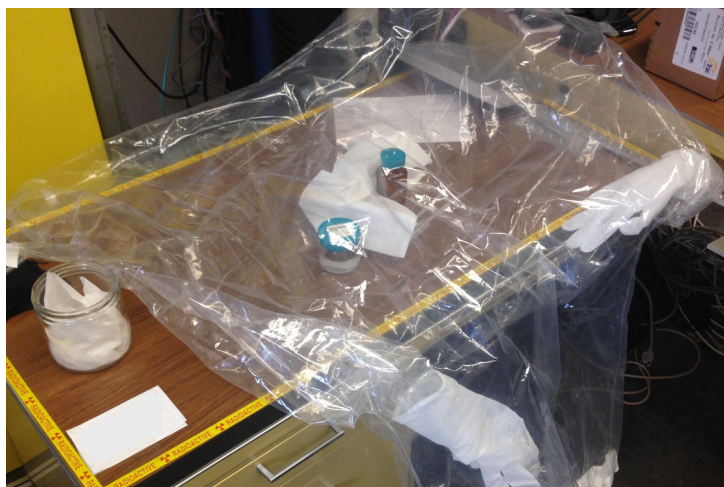


Figure 5.12: A sealed desktop glove bag for polonium deposition.

The quantity of adhesion promoter was chosen so as to minimize interference of the chemical layer with the ^{210}Po decays. The TMS-ED3A (CAS #128850-89-5, Gelest, 35% by weight) was further diluted with DI water to 0.008% by weight, such that 1 drop ($\approx 1/16$ ml) would create a ≈ 50 nm thick film over the area of the drop (roughly 0.5 cm^2).

The PIN diode was prepared by swabbing the silicon surface with hydrogen peroxide (JT Baker MEMS grade diluted with DI water to 3% by weight). To prevent accidental environmental release of polonium, the diode and deposition materials are placed in a clean desktop glove bag (Fig. 5.12). The bag is then sealed and inflated with nitrogen gas. The glove bag operator applies two droplets of the polonium solution on the center of the PIN diode face, followed by a single droplet of the adhesion promoter. After retrieving the PIN

diode, gentle heat is applied to accelerate the drying process and bake the PIN surface.

Multiple tests were done following the deposition procedure to assess the α decay rate. An initial rate assessment was done with a survey meter, which showed rates < 10 Bq. Since the PIN is itself an α detector, an external charge amplification setup was also used, with separately both an oscilloscope and a CAEN digitizer to perform α counting on the signal from the biased PIN diode. These tests yielded overall α rates of $\approx 1 - 5$ Bq.

The ultimate goal of the procedure is to ensure adhesion in LXe without contaminating the detector space. Therefore, the rate of the PIN source was found before and after a long soak in warm cyclohexane in order to check for dissolution of the source layer; there was no detectable change in the source activity. Cyclohexane actually shares many solvent properties with Xe, which is evidenced by the similarity of their solubility coefficients and other chemical properties (e.g. dielectric constant) [34, 85, 109, 204], but is infinitely cheaper and more convenient to work with.

5.4.3 A High-Voltage PIN-Cathode Assembly

For this experiment, we have created a special cathode that allows for biasing and readout of the coated PIN source while simultaneously providing the necessary HV to produce drift fields in the TPC.

The PIN diode is floated at high voltage on a solid copper cathode using a voltage divider circuit which maintains a fixed fraction of the cathode bias across the PIN (see Fig. 5.13). This circuit board is in direct contact with both the cathode and the PIN, with one lead of the PIN diode at high voltage and the other lead at a voltage determined by a parallel resistor. The remaining high voltage is shunted to ground via a $1\text{ G}\Omega$ resistor, and decoupling capacitors decouple the charge signal on either side of the PIN diode.

The various resistance and capacitance values in the circuit are optimized using Spice simulations, in order to ensure the PIN charge signal is not adversely affected. However, the parallel resistor is chosen based on high voltage constraints. To achieve reasonable drift fields in the ≈ 1.8 cm LXe drift length, a maximum cathode voltage of -1.6 kV is used, far

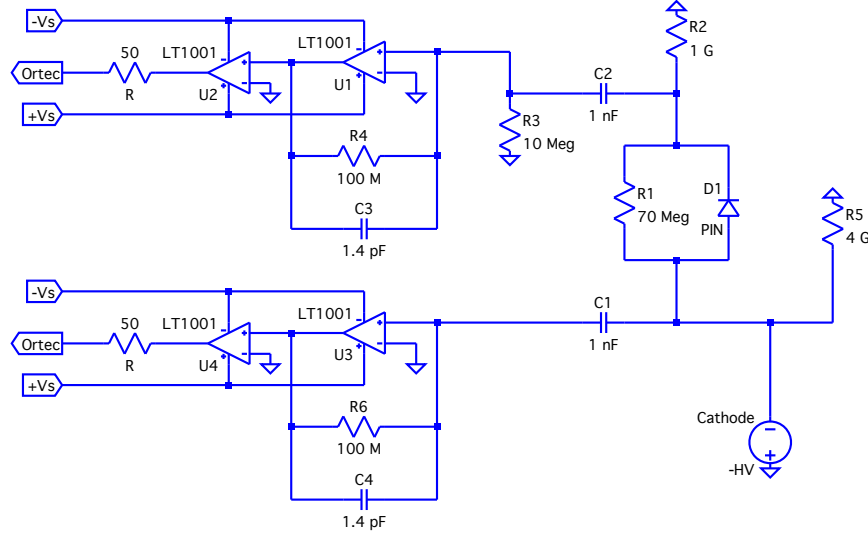


Figure 5.13: The PIN circuit diagram in LTspice, with the $4\text{ G}\Omega$ representing the TPC resistor chain and the two left-most blocks representing the Cremat amplification circuits.

surpassing the 100 V maximum reverse voltage rating of the diode [175]. The voltage divider is therefore designed to drop 1/16 of the cathode voltage across the PIN diode. A PIN bias range of 25-100 V corresponds to a cathode operational range of 400-1600 V.

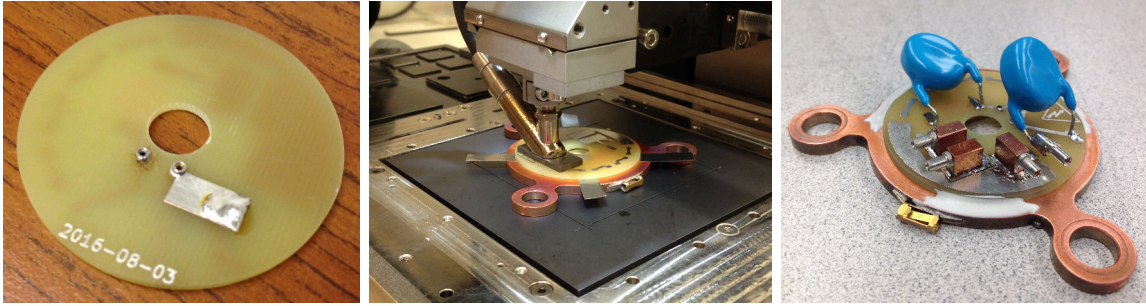


Figure 5.14: (Left) HV solder trace for the copper side of the PIN circuit. (Middle) Process of soldering using the flip-chip bonder. (Right) The cathode backside after partial population of the PIN circuit.

The PIN-cathode assembly is constructed by using a flip-chip bonder to solder a trace on the PIN circuit board directly to the copper cathode (Fig. 5.14). Resistors, decoupling capacitors, and custom cable connectors are then soldered onto the backside of the circuit. To prevent the circuit board components from contaminating the LXe, the circuit is potted

with vacuum-grade epoxy in the final stage of assembly.

The PIN diode used is a Hamamatsu S3590-09, an unsealed silicon chip seated on a ceramic base (see Fig. 5.15). The chip's depletion region is $\approx 300 \mu\text{m}$ thick [175], ample for ensuring full energy deposition by an incident α .

Before final assembly of the TPC, all components (with the exception of the PIN diode, which is prepared separately) are subjected to thorough cleaning to avoid contamination of the Xe. The majority of components undergo multiple rounds of soaking in an ultrasonic bath; they are immersed in a beaker of acetone and sonicated for 15 minutes, then the process is repeated with a beaker of isopropanol. The remaining components, which are either too bulky or too sensitive, are gently wiped down with the solvents. Exposure to dusty and dirty air are minimized where possible, and handling is done with gloves and face-masks.

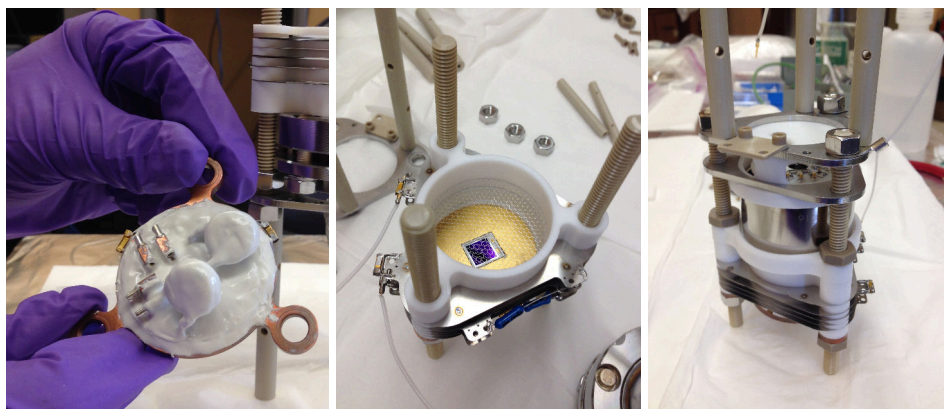


Figure 5.15: (Left) The epoxied circuit on the backside of the cathode. (Middle) The PIN-mounted cathode facing up into the TPC, PMT removed. (Right) The TPC almost fully assembled, with PMT mounted.

5.5 The DAX Infrastructure

5.5.1 Outer Vacuum, Thermosiphon and Cryogenics

A major component of building a liquid Xe system is building a cryogenic system for cooling and liquefying the Xe. This requires substantial infrastructure to maintain vacuum for providing thermal insulation from the warm lab environment.

In Fig. 5.16, we present the phase diagram for Xe. Such a plot is taped to the wall in many a lab, as it shows the pressure and temperature corresponding to Xe condensation. Xenon has a triple point at $T \approx 161$ K and $P \approx 0.8$ bar [211], where Xe exists in all 3 phases, and to liquefy Xe a temperature above this triple point and pressure above the saturation curve (liquid-gas boundary) must be maintained. Therefore, given the desired range for operational detector pressures of between 1-3 bar ($\approx 1 - 3$ atm), operational temperatures are typically in the range of $\approx 165 - 180$ K.

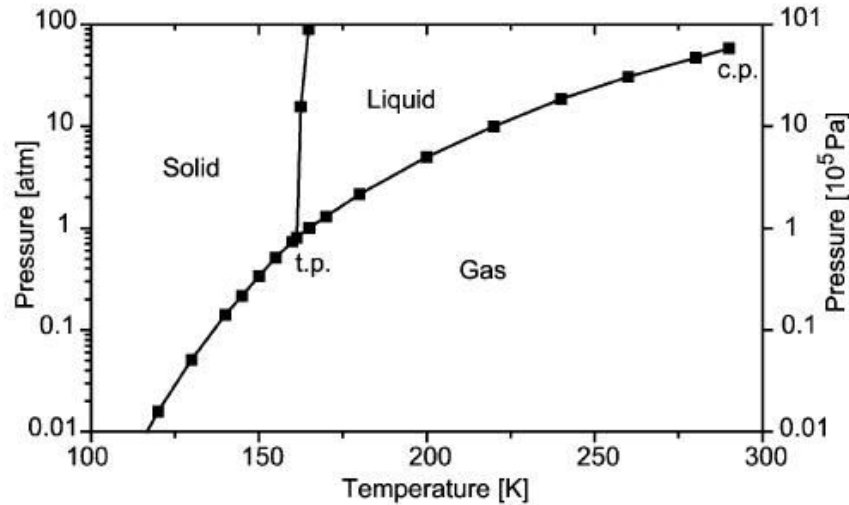


Figure 5.16: A log-scale Xe phase diagram, from [65].

To condense Xe, we use a heat-pipe thermosiphon system to provide the necessary cooling power to absorb heat from the warm Xe gas via a cold head. The cold head is a copper mass that extends into the Xe vessel, and is connected via two VCR lines to a nitrogen condenser located in a tower above the Xe space. The condenser is a chamber in contact with a thermal

bath of liquid nitrogen (LN). When nitrogen gas is injected into the thermosiphon loop and the upper dewar is filled with LN, the gas in the loop condenses, falls down to the cold head, evaporates from cold head heat transfer, and re-condenses in a continuing cycle.

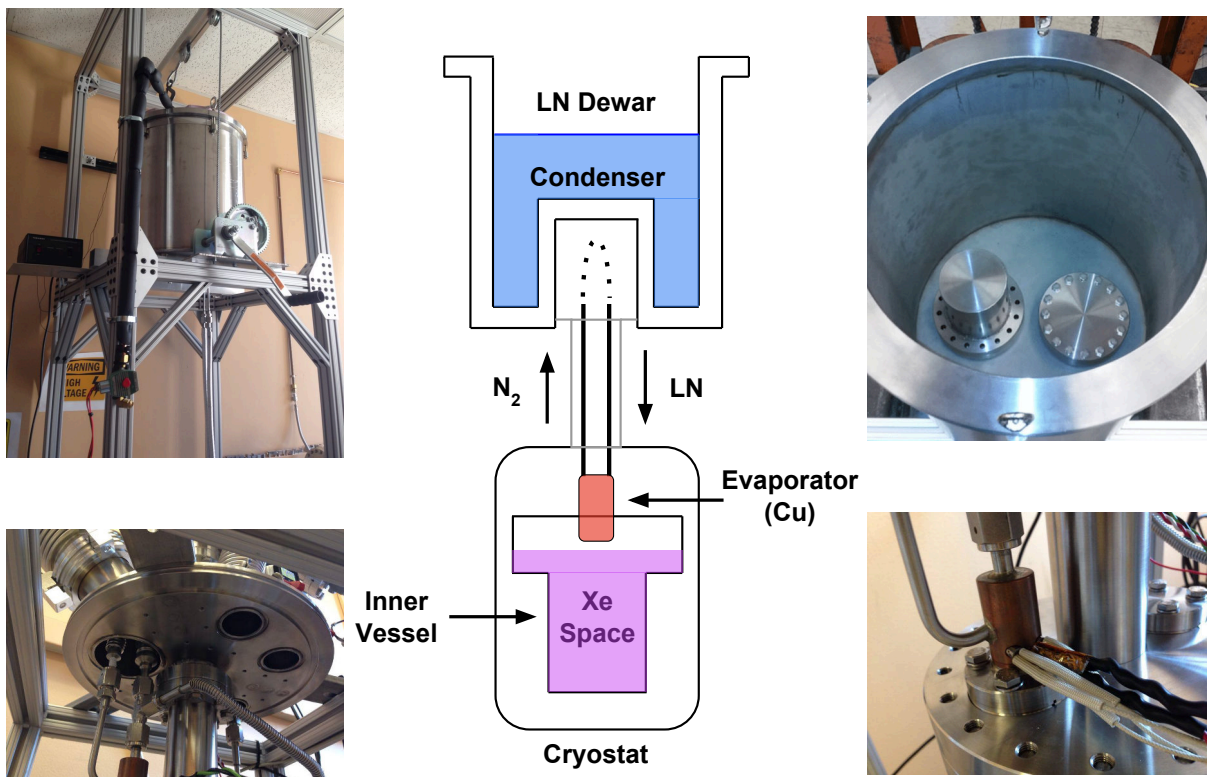


Figure 5.17: (Center) A basic diagram of heat-pipe thermosiphon operation for condensing xenon. (Top left, right) Thermosiphon tower and LN dewar, with the outside of the nitrogen condenser visible. (Bottom left, right) Nitrogen VCR lines coming down through the enclosing vacuum hose and attaching to the copper coldhead, and a closeup of the coldhead with PT-100 and heaters in place.

As the warm Xe gas transfers heat into the cold head, it condenses and fills the Xe space with liquid. The ability to condense Xe depends on the cooling power and stability of the thermosiphon system, which is controlled by the total amount of nitrogen in the cold head loop. The temperature of the cold head can be very finely controlled using a Cryocon Model 26 temperature controller, which reads a PT-100 temperature sensor and uses a PID loop to adjust the power output on a set of cold head heaters. The thermosiphon, outer vacuum

system, and cold head are shown in Fig. 5.17.

5.5.2 The Xenon Cryostat and Feedthroughs

Our Xe space consists of an upper “warm” end and a lower “cold” end. The warm end is known as the “Medusa” since it has many attached feedthrough ports and allows for breakout of the various HV and signal lines running to devices in the Xe space. A steel tube extends down from the warm end into the insulating vacuum space and meets the ceiling of our cold Xe space. The “inner can” is then raised to meet this steel flange, thereby enclosing the Xe volume with a system of exclusively CF vacuum-tight flanges.



Figure 5.18: (Left) The Medusa head mounted on a T-slot frame, with cabling pipe extending down into the cold space. (Right) Inner vessel can sealed up, enclosing the Xe space.

Once the inner can is bolted onto the Xe space assembly, the outer vacuum can is raised to the large flange flush with the top of the T-slot frame (see Fig. 5.18). A seal is created at the LF gasket using KF-style clamps. This outer vacuum can then forms a continuous space with the upper thermosiphon dewar via a large flex hose surrounding the VCR nitrogen lines.

Pfeiffer HiCube turbo-molecular pumps are used to pump out both the inner and outer

spaces. To ensure vacuum tightness of the Xe space, it is pumped down to a level of at least $\approx 10^{-6}$ mbar before a Xe fill.

5.5.3 Xenon Circulation System

Xenon must be recirculated during dual-phase operation for constant purification, as outgassing and contamination by internal components increases the presence of electronegative impurities. A large concentration of impurities leads to capture of drifting electrons, which reduces the electron lifetime and attenuate charge signals. In the DAX experiment, a commercial SAES Monotorr heated getter is used to remove major impurities to < 1 ppb [197].

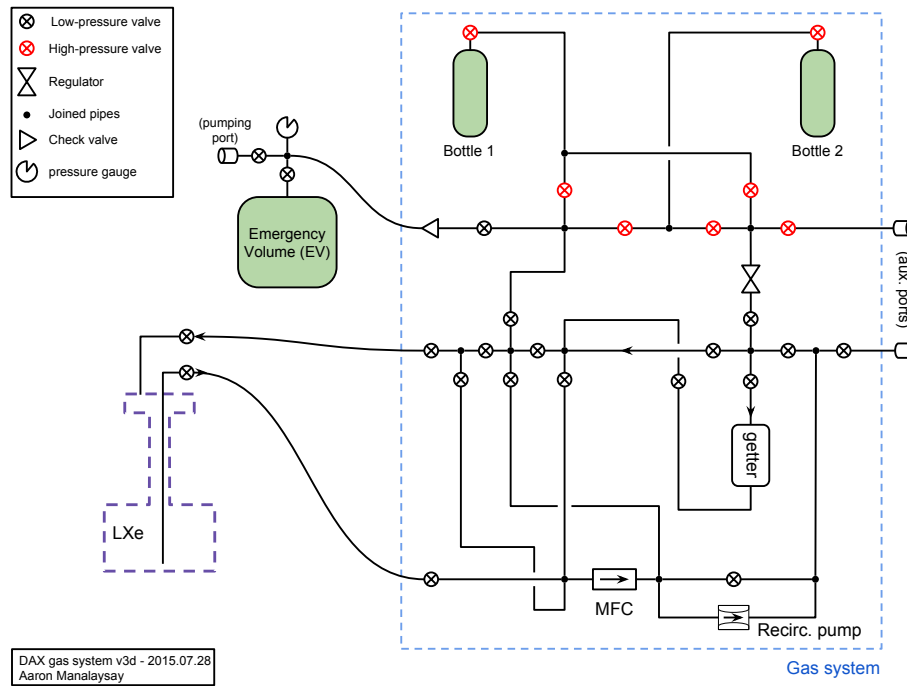


Figure 5.19: The DAX circulation system, courtesy of Aaron Manalaysay.

In order to recirculate and maintain a steady liquid level, a method for drawing out Xe and regulating the recirculation flow is needed. Fig. 5.19 shows a diagram of the gas circulation system, which provides multiple fill and recovery paths. A siphon tube extends down nearly to the bottom of the inner vessel, and a recirculation pump draws liquid up the tube which then vaporizes at the warm end. This Xe then flows through a MKS GM50A mass

flow controller (MFC), which restricts the Xe flow. This purified Xe then passes through the getter and follows a return path to the inner vessel.

The system contains two Xe bottles, one for holding a Xe reserve and one for holding the necessary Xe for filling. An additional Xe recovery vessel (called the “Emergency Volume”, or EV), is hooked into the circulation system via a one-way 3 bar differential valve for emergency recovery in the case of dangerous pressure build-up.

We use a cryo-pumping procedure to recover Xe, which involves surrounding the Xe bottle with a suspended dewar of LN, which depressurizes the bottle to vacuum and freezes the contents. We can then draw Xe back into the bottle by opening this vacuum to the detector space.

5.5.4 A Slow Control Database and Monitoring System

Operations in the DAX lab require the simultaneous monitoring of many devices. We have developed a slow control system (SC) for storing and retrieving sensor data in a convenient format, which also serves as an alert system for notifications in case detector conditions change unexpectedly.

The slow control system is run as an Ubuntu service via the Upstart framework, allowing for the operating system to run the slow control program and automatically restart the process upon reboot. System logs are stored, and alerts are sent if the process fails to restart multiple times. This system process runs a Python slow control script, which communicates over serial and ethernet connections to various laboratory devices and stores those values in a MySQL database via the PyMySQL library.

The MySQL database, called “DAX_SC”, contains a table for each lab device. In general, each device (table) has associated attributes (columns), with an entry (row) for each time sample. Therefore, if a device needs to be added, it be added as a new table without modification of the existing data structure. Tables exist for the temperature readouts of the cold head and inner Xe space, the heater power output of the Crycon, the pressures of the outer vacuum space and Xe space, the recirculation flow rate through the MFC, and the

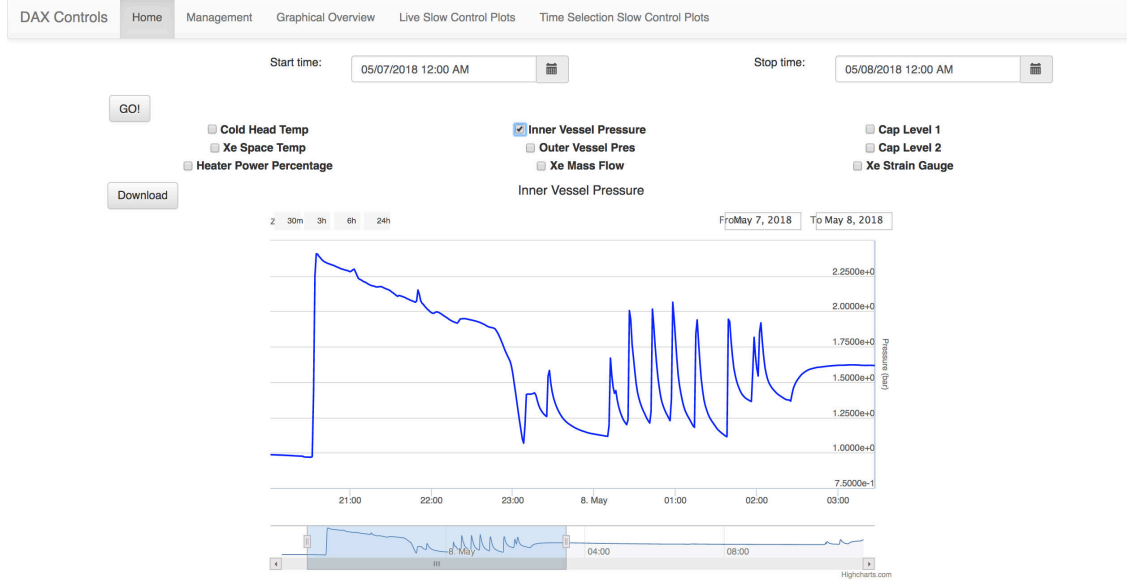


Figure 5.20: A screenshot of live plotting on the slow control website. Shown is a time selection of Xe space pressure gauge readings.

capacitances of the liquid level meters.

Through master-slave replication, the SC database is kept in sync between the master server (lab computer) and slave (remote web server). This allows the remote web server to query values from a local copy of the database and update plots on the slow control website. This website is generated using a Python Flask application, along with Javascript libraries such as JQuery and Highcharts to allow dynamic interfacing with the online plots such as zooming and time selection capabilities.

5.6 Data Acquisition and Processing

As previously mentioned, the internal PIN diode and PMT signals are broken out at the warm end feedthroughs and amplified. These amplified signals are then fed into separate channels on a DDC-10 digitizer unit. To avoid bias, and because the PIN diode would serve as a trigger for ^{210}Po decays in the analysis, datasets were taken with different trigger settings for later comparison. In one scenario, the DDC was set to trigger on the smallest possible

signals from the high gain channel of the PMT while avoiding baseline noise. In the other, the DDC was set to trigger on the PIN signal to increase the relative rate of ^{206}Pb events.

The DDC buffers the input waveforms so that upon a triggered event, it captures a user-specified number of samples before and after the trigger and records the waveform to a binary output file, all while tabulating the dead time due to these operations. The DDC uses a differential threshold, rather than an absolute threshold, to automatically account for baseline shifts and minimize triggers on noise.

A data processing framework called ADAX was developed to process the binary data files and generate useful reduced quantities through waveform analysis. This includes a pulse-finding and signal classification code which identifies S1 and S2 signals, as well as charge signals from the PIN diode. The latest version of this package, including schemes for S1/S2 classification, will be discussed in detail in Sec. 7.3.

5.7 Evaluation of the Triggered Source in LXe

The PIN diode source was implemented in two separate trials of dual-phase TPC operation, about 16 days and 9 days of Xe recirculation respectively.

The signal size of α particles detected in the PIN diode, as measured from both pulse height and integrated pulse area (Fig. 5.22), is consistent throughout recirculation (and not significantly altered compared to prior room temperature testing). This demonstrates that the diode's performance is not compromised when immersed in LXe at temperatures down to ≈ 165 K.

In addition, in datasets where the DDC was triggered by the PIN signal, the rate of α signals in the PIN diode is measured to be 1.1 Hz within 5% fluctuations over the course of operations. With the digitizer set to trigger on the PMT channel, the rate of α events in the acquisition is still consistent across both runs to within 10%. The persistence of the α rate implies that the source was not degraded during either run, validating our deposition procedure.

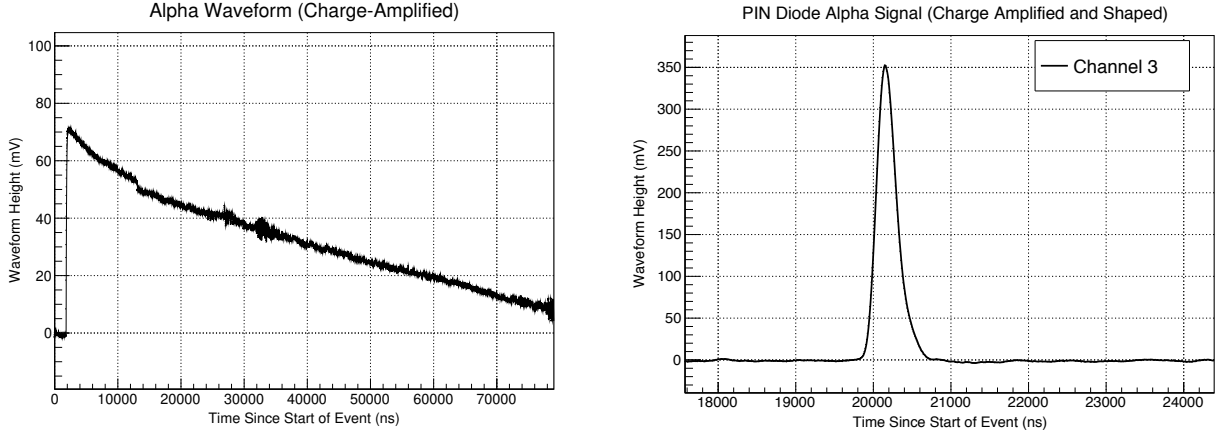


Figure 5.21: (Left) An example PIN alpha signal waveform as directly output by the charge amplifier. (Right) An alpha signal after additional shaping.

The signal-to-noise ratio of our α signals is outstanding, as can be seen from a typical PIN waveform (Fig. 5.21). While charge amplification provides the necessary signal gain ($\approx 1.4 \text{ V/pC}$) [81], shaping reduces the time constant of the pulse from $\approx 100 \mu\text{s}$ to $\approx 1 \mu\text{s}$.

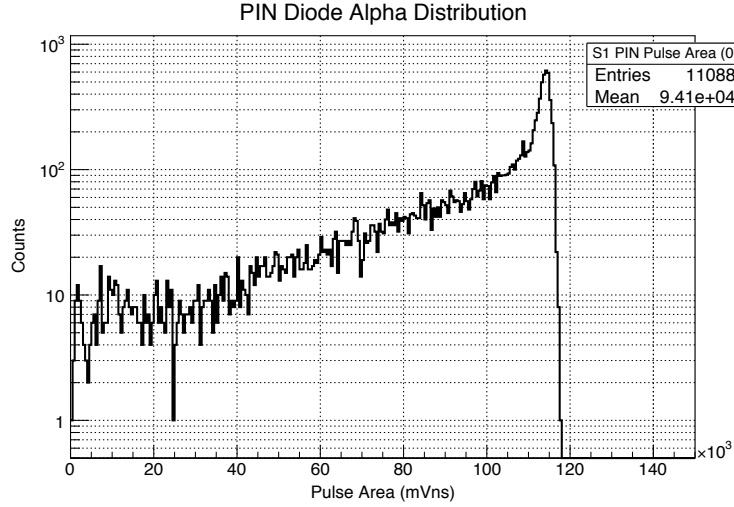


Figure 5.22: A distribution of integrated pulse areas for all α signals detected by the PIN source, with a high resolution peak for the full deposition of 5.3 MeV.

Furthermore, we can resolve a 5.3 MeV peak from the signal spectrum (shown in integrated pulse area), while the long shoulder includes α events with incomplete charge collec-

tion and partial energy deposition.

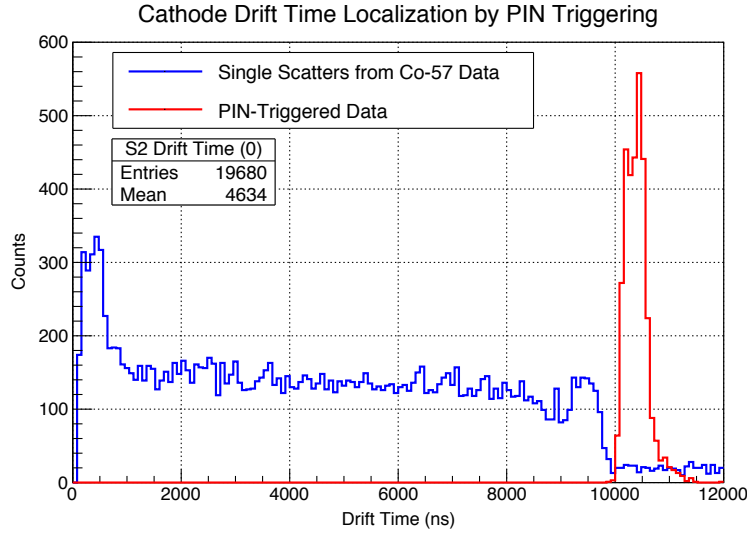


Figure 5.23: A comparison of the drift time distributions for candidate ^{206}Pb events and single-scatter events from an external ^{57}Co source.

In order to identify ^{206}Pb events, some cleanliness cuts are made in post-processing. Once a PIN-triggered event has been found (i.e. a charge pulse is identified in the PIN channel), we make two additional cuts. The first is on the size of the charge signal in the PIN, which ensures that we are selecting events where the ^{206}Pb has the fullest energy deposition in the LXe and minimizes surface effects. The second cut is on the drift time between the S1 and the S2, since we desire only events that are truly localized to the cathode.

By simply implementing the first cut and selecting α signals with pulse area greater than 1.1×10^5 mV·ns, we see from Fig. 5.23 that the drift time is already tightly constrained to the cathode. This is encouraging, as it proves that the PIN-triggering method automatically localizes the source and there is little background contamination.

To verify the location of the cathode, an external ^{57}Co was used to collect 122 keV γ events throughout the drift region at the same drift field. A simple selection cut on single scatters (1 S1, 1 S2) is made. The reconstructed drift time distribution is physically sensible, given that events at highest drift are suppressed due to field effects in the periphery.

In Fig. 5.24, the time difference between the α PIN signal and S1 PMT signal is shown

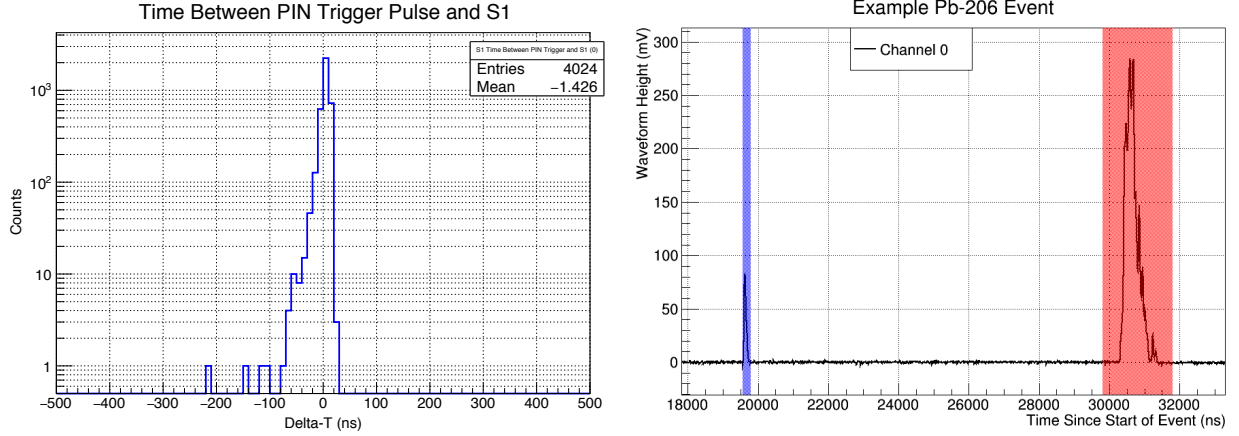


Figure 5.24: (Left) Tight time correlation between PIN diode α signals and primary scintillation (S1) signals seen by the PMT, after cutting on the main α peak. (Right) Candidate ^{206}Pb event obtained by α trigger, with blue window indicating the S1 signal and the red indicating the electroluminescence signal (S2).

(for events with both present). It is clear that PIN-triggered events are highly time-correlated with the S1 signals seen by the PMT; the majority of S1 signals falling within 100 ns of the α trigger. A candidate ^{206}Pb nuclear recoil signal from this population is shown.

These results show the successful implementation of a persistent, triggered source of ^{206}Pb nuclei in a dual-phase Xe TPC. While such a device may be useful for future experiments who desire *in situ* monitoring of such backgrounds, our constraint of operating such a device on the cathode poses problems for direct characterization of the ^{206}Pb yields.

In such a high field region, the electrostatics have to be very finely modeled to understand the charge collection. This is especially difficult with the PIN-cathode assembly, where the decoupling circuit and built-in electrostatics of the PIN device introduce significant unknowns into the local field profile. In addition, light collection is suppressed in such a configuration, since it is well-known that light collection (particularly for S1 signals) is largely concentrated in the bottom PMTs due to optical effects at the liquid-gas interface [29, 40].

Other methods are needed to properly investigate the light and charge yields of these nuclear recoils, and these will be discussed in the next two chapters of this thesis.

Chapter 6

Modeling a New DAX TPC

As discussed in the previous section, careful studies of the Xe response to ^{206}Pb nuclear recoils required a redesign of the DAX TPC. These changes, including the creation of a new set of localized sources, will be discussed in this chapter. In addition, we will discuss the results of various detector simulations, which were performed to assess the viability of this new paradigm and inform key aspects of the experiment.

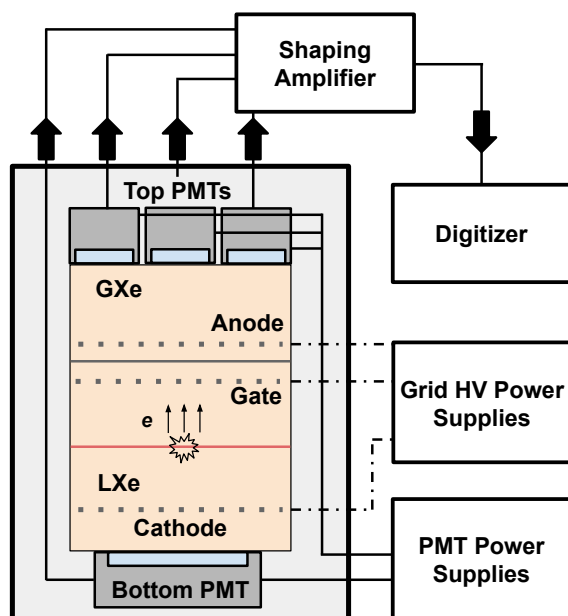


Figure 6.1: A simple schematic of the new DAX TPC configuration.

6.1 A New Paradigm for Measuring ^{206}Pb

In the absence of direct α tagging with a PIN diode, full 3-dimensional localization of the source is required to exclude interfering backgrounds. In order to easily isolate source events and minimize field effects, we implement a highly localized source in the center of the drift region (see Fig. 6.1). Using an array of PMTs, we may then perform position reconstruction to fiducialize the source and identify ^{206}Pb nuclear recoils.

Suspending the source in the middle of the drift region requires a low-profile substrate, to avoid interfering with the drift fields or accumulating drifted charge from events in the lower half. Thus, for our substrate we use a thin rod (with a diameter of ~ 1 mm) spanning the TPC drift region.

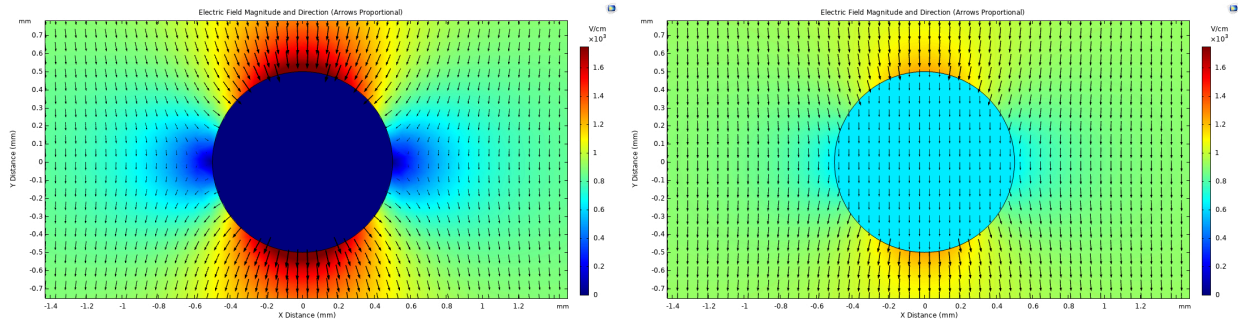


Figure 6.2: COMSOL simulations of a stainless steel rod (left) and a fused silica rod (right) immersed in a uniform drift field, as described in the text.

We weigh a number of important considerations when choosing our substrate material. First, we consider how the source rod will affect electric fields in the detector. Using the AC/DC module of the COMSOL Multiphysics[®] software package, simple simulations were performed with both insulating and conducting rods suspended in LXe in a uniform drift field of ≈ 1 kV/cm (see Sec. 6.4 for details on simulation parameters).

Simulation results for the conducting rod raise concerns. In Fig. 6.2, we see that even for an ideal scenario with a smooth stainless steel rod at a floating potential, there are very high fields near the surface, with variations of at least $\approx 100\%$. In reality, any microscopic surface variation in a conductor (i.e. sharp points or scuffs) creates more extreme local

field variations due to the crowding of field lines, as in the “lightning-rod effect” [94, 105]. Furthermore, simulations show that even small deviations from this floating voltage result in highly asymmetric and unstable fields in the neighborhood of the rod. This is especially concerning since it has neighboring high voltage components near the edge of the detector.

Insulating materials are highly constrained, however, since the chemistry of our source deposition procedure relies on a glassy or metallic surface for proper adhesion; this rules out plastics such as PTFE or PEEK. Fused silica has a number of desirable properties that make it an ideal substrate. It has a very smooth surface, which minimizes local field variations. It has minimal impurities, low thermal expansion, and relatively high tensile strength [123, 218]. In general, it also has excellent optical properties, with some types having high transmission of photons deep into the UV range.

Though fused silica may luminesce from strong photo-excitation [55, 101, 110, 126, 232, 245], there is no interfering component detected in our samples or specified by the manufacturer of our particular material [122]. Fused silica is also known to become easily charged [49, 59, 87, 118, 127, 233], however given proper passivation and discharging of the substrate, we can minimize this risk. Localized charge accumulation on the rod would then be limited to drifted electrons within the TPC, which is not of great concern given the low expectation of background radiation in the vicinity of the source. Furthermore, our COMSOL simulations show that $\mathcal{O}(10\text{ mC/m}^2)$ of surface charge is required on the fused silica rod to noticeably affect the field profile, which is substantial even when compared with intentional charging experiments [59, 118, 127].

Fused silica was chosen as the substrate for our new sources. In addition to the new source, many other improvements were made in the re-design of the TPC:

- The 2-inch PMT is placed at the bottom of the TPC to maximize S1 light collection.
- 3 1-inch square PMTs (Hamamatsu R8520-406) form an array at the top of the TPC for position reconstruction using S2 signals.
- The solid copper cathode from our PIN diode configuration is replaced with a mesh

grid above the bottom PMT, reducing electron backgrounds from photoionization.

- Smoother, lower-profile solder-mount pin sockets are used as HV connectors for grid and FSR cables, as well as for the resistor chain. This reduces sharp points which can cause sparking due to local high field regions (see Sec. 6.4.5).
- Multiple liquid level meters are mechanically fixed to the gate-anode gap using a newly designed PTFE spacer, rather than being suspended by PEEK rods; this ensures proper alignment of the plates with the extraction region.

6.2 Local Energy Depositions of Heavy Recoil Ions

In our new paradigm, a rod is coated with a layer of deposited source. It is not clear from the outset how the local microphysics of a ^{210}Po decay is affected by this geometry, including the source layer itself. From previous development of thin heavy ion sources, it is understood that contamination, surface roughness, and layer thickness can cause significant losses in the efficiency for measuring recoil ions [177]. It is therefore important to understand how our proposed source geometry will affect the observable energy spectrum.

6.2.1 Particle Tracking with GEANT4 and BACCARAT

The GEANT4 simulation software uses physics and materials libraries to probabilistically track particles as they traverse various media. This is useful for understanding how particles deposit energy for a given detector geometry, taking into account variations due to kinematics and different material properties. BACCARAT (**B**asically **A** **C**omponent-**C**entric **A**nalog **R**esponse to **A**ny **T**hing), initially called “LUXSim” [9], is a GEANT4 implementation specifically developed for LUX. It pre-defines many of the materials and radioactive sources commonly used in dual-phase Xe detectors and uses a new set of classes which aid in geometry construction within GEANT4. BACCARAT is a tool with ongoing development within the LZ collaboration, and is generally applicable to other Xe experiments.

We can use BACCARAT to build a simple geometry for our proposed heavy ion source and study how the simulation parameters affect the resulting energy distribution. This is important, as only energy depositions in the Xe itself will result in measurable light and charge yields for characterization of the nuclear recoils.

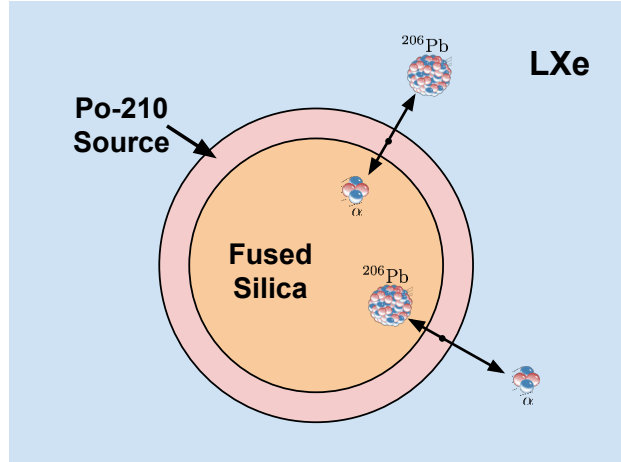


Figure 6.3: A simple illustration of the fused silica source geometry used in GEANT4.

The source is constructed in BACCARAT as a cylindrical quartz rod coated with a cylindrical shell of dried adhesion promoter (containing the source), all immersed in an effectively infinite volume of LXe (Fig. 6.3). The adhesion promoter is created as a new GEANT4 material based on the chemical formula $C_{14}H_{25}N_2NA_3O_9SI$, and its density is approximated as that of glass based on its amorphous solid structure.

The BACCARAT package has built-in source generators which reference radioactive decay tables, as well as physics libraries which model energy loss of the resulting particles in matter. These features are used to generate a million ^{210}Po decays randomly throughout the source layer. We repeat such a simulation for various thicknesses of the adhesion promoter layer, ranging from 1 nm to 20 nm. Each event results in isotropically-generated back-to-back particles: a 5.3 MeV α particle and a 103 keV ^{206}Pb nucleus. Note that the daughter nuclei are emitted as neutral particles in GEANT, whose interactions are governed by various low energy nuclear recoil models in the physics list, including the “G4ScreenedNuclearRecoil” class which deals with energy loss associated with Coulomb collisions between nuclei. This

may not be a truly accurate representation of the recoil spectrum; for more discussion of charged ion daughters, see Sec. 6.2.2.

The range of α particles in various materials is well-known, so one check of our geometry is to inspect the energy distribution for these particles and their track length in each medium. The BACCARAT simulation output contains the “steps” in a particle track at which energy is deposited, which include information such as the position of the particle and the material of the interaction volume at that step. In code, we loop over the steps in each particle track in each event, summing the energy depositions and distance traversed in each material for the particle track.

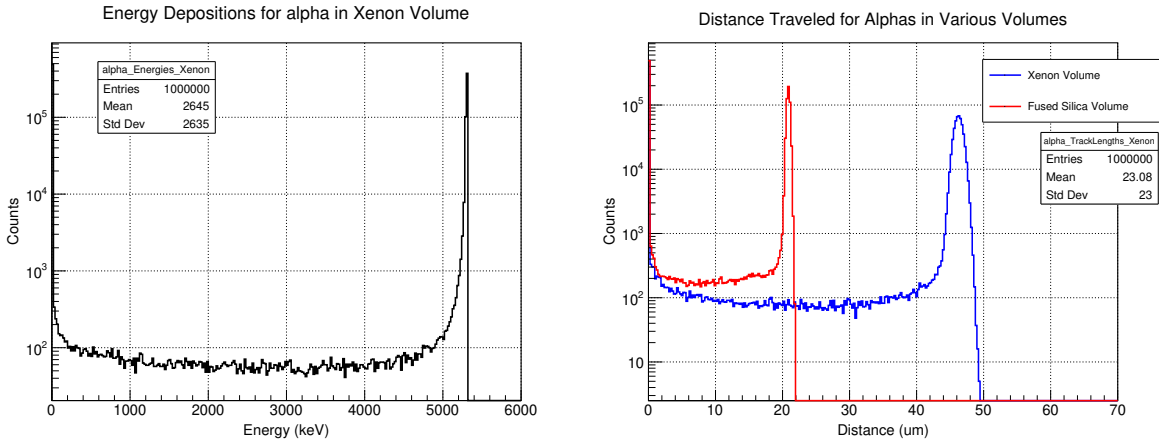


Figure 6.4: (Left) Total energy deposited by α particles in the LXe. (Right) Cumulative distance traveled by the α particles in the LXe (blue) and quartz (red).

Shown in Fig. 6.4 is the energy deposited in Xe for α particles generated in a 20 nm layer of adhesion promoter, as well as the total distance traveled in the Xe and quartz (no α particles are stopped in the adhesion promoter). The results are quite reasonable; α particles are highly likely to deposit their entire energy in either the quartz or the LXe, and travel distances in each medium that agree with the literature ($\approx 20 \mu\text{m}$ in quartz [68] and $\approx 45 \mu\text{m}$ in LXe [141]). This result tells us an additional important fact: the relative rate of events where the α deposits an intermediate energy in the LXe (other than 0 or 5.3 MeV) is almost negligible, so there should be a low expectation for events where both the α and

^{206}Pb produce comparable energy depositions and skew our yield measurements.

In order to optimize our resolution of the light and charge yields for the ^{206}Pb nuclei, we want our nuclear recoils to be as close to mono-energetic as possible. We see from Fig. 6.5 that even for a 20 nm layer, the energy distribution is highly smeared and would limit us to an endpoint measurement; a 1 nm layer is ideal, giving a tight energy peak at 103 keV.

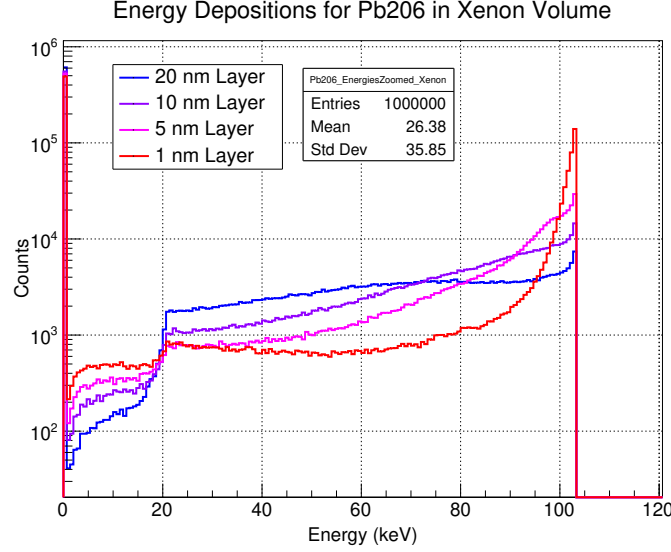


Figure 6.5: Deposited energy distribution for ^{206}Pb nuclei in the LXe medium for various adhesion promoter layer thicknesses.

These effects can be understood by inspecting the track lengths of the nuclei in the various media. In Fig. 6.6, results are shown for two different thicknesses of the source layer. With a 20 nm layer, the ^{206}Pb ion dies a significant fraction of the time in the source layer itself or after traveling just a short distance into the LXe or quartz. The flat-top distribution up to 20 nm in the source layer is due to nuclei being emitted at glancing angles, being completely absorbed and never depositing energy in another medium. With a 1 nm layer, the nucleus clearly penetrates further on average into the quartz (≈ 30 nm) and LXe (≈ 50 nm). These numbers roughly agree with existing literature [83, 98, 184, 209, 244], however there is still limited knowledge of how ^{206}Pb ions travel in LXe and the GEANT4 physics models used here should be met with healthy skepticism.

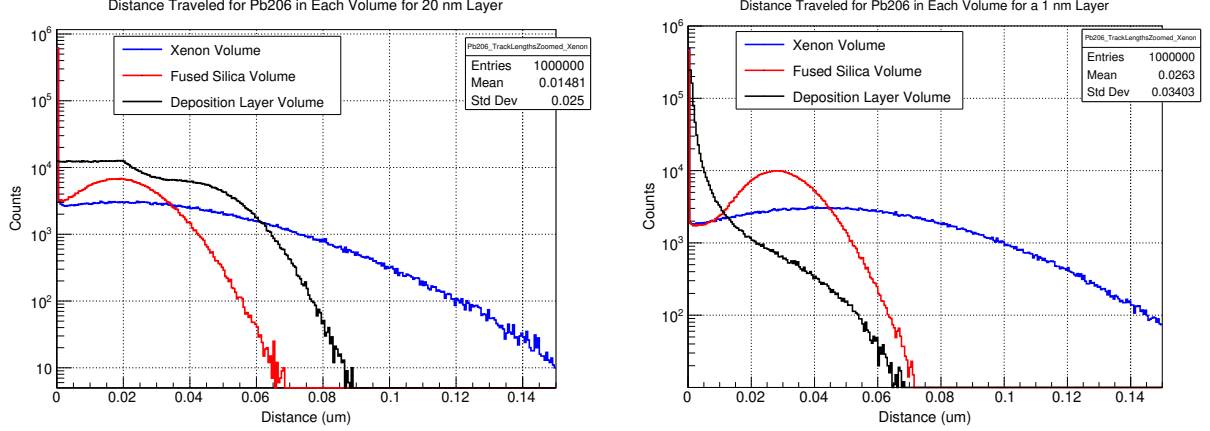


Figure 6.6: Cumulative distance traveled by ^{206}Pb nuclei in each volume for a 20 nm thick source layer (left) and a 1 nm layer (right).

These simulations have important implications for our experiment. Since the energy distribution is highly dependent on the thickness of the source layer itself, it is crucial that we minimize this layer by carefully planning the source deposition chemistry. It should be noted even a mono-energetic source may not be well-represented in the signal distribution, since it is unclear how charge loss and other surface effects affect the observed charge yield.

6.2.2 Charge States of Heavy Ions in LXe

The uncertainties in our energy deposition model warrant additional discussion, since in actuality nuclear decay daughters are not necessarily neutral. A recoil daughter ion has a charge state which determines how it loses energy in matter, and the probabilistic charge state distribution is dependent on both the surrounding medium and the decay process.

Naively, the immediate charge of a recoil ion resulting from either α or β decay would simply depend on the charge lost (+2 or -1), however the picture is complicated by the rearrangement of the electron cloud. It is understood that the dominant primary ionization process during nuclear decays is “electron shake-off”, where the innermost shell electrons (K , L , M) are shed due to the sudden change in the Coulomb potential and the perturbation of the electron cloud by the recoiling nuclei [80, 181, 182]. Additionally, the resulting inner

shell vacancies induce Auger cascades which lead to further X-ray and electron emission.

Careful studies of β^+ decays have been done to leverage the final charge states of recoil ions for investigations of weak interactions [80, 206], and have shed further light on these atomic processes. Regardless of the decay mode, negatively charged recoil ions are either highly unstable or not emitted; in fact, they are usually positively charged, with the branching ratio generally decreasing for higher charge [206].

For an α decay, ≥ 2 atomic electrons are given up by the heavy daughter, resulting in a positive charge that is eventually neutralized by electron pickup in the medium. Recent results in the EXO-200 LXe detector provided the first measurement of α -decay daughter ion fractions in a noble liquid, using delayed coincidence of ^{218}Po with its parent ^{222}Rn decay as a charge-independent tagging mechanism [31]. These Rn decays were found to result in singly-charged $^{218}\text{Po}^+$ ions $\approx 50\%$ of the time, with the remaining nuclei being neutral. Most existing data pertains to light or high energy ions, making comparison difficult; however, this measurement is found to be within $\approx 10\%$ of ion fractions for ^{218}Po measured in some noble gases (Ar and He) at atmospheric pressure.

Available data indicate significant variation in the charge distribution for different recoil species in different media. Since the charge state branching ratios of ^{206}Pb are not well-measured in LXe, and charged states may effectively skew the resulting energy distribution, we must consider this as a systematic uncertainty in our model.

6.3 Understanding Light Collection in the TPC

In addition to energy deposition simulations, GEANT4 and BACCARAT is used to build a simplified geometry for the DAX TPC in order to simulate the optical performance. While material properties, e.g. photon reflectivities at VUV wavelengths, cannot all be precisely known without extensive side measurements, it is still very useful to develop a detector model for simulating light collection and cross-checking with experimental results. “Photon bomb” simulations allow us to estimate the geometric light collection efficiency (LCE) in the

drift and extraction regions, as well as optimize our position reconstruction using the known Monte Carlo values.

Detector components in BACCARAT must be built using simpler GEANT4 shapes, which may be combined using boolean operations such as intersection, union, and subtraction. An arbitrary part may require many constituent shapes and an unfeasible amount of code; this limits the complexity of our BACCARAT TPC model. For light collection simulations, we care almost exclusively about the interior optical surfaces of the TPC, so we truncate parts that extend beyond the active region.

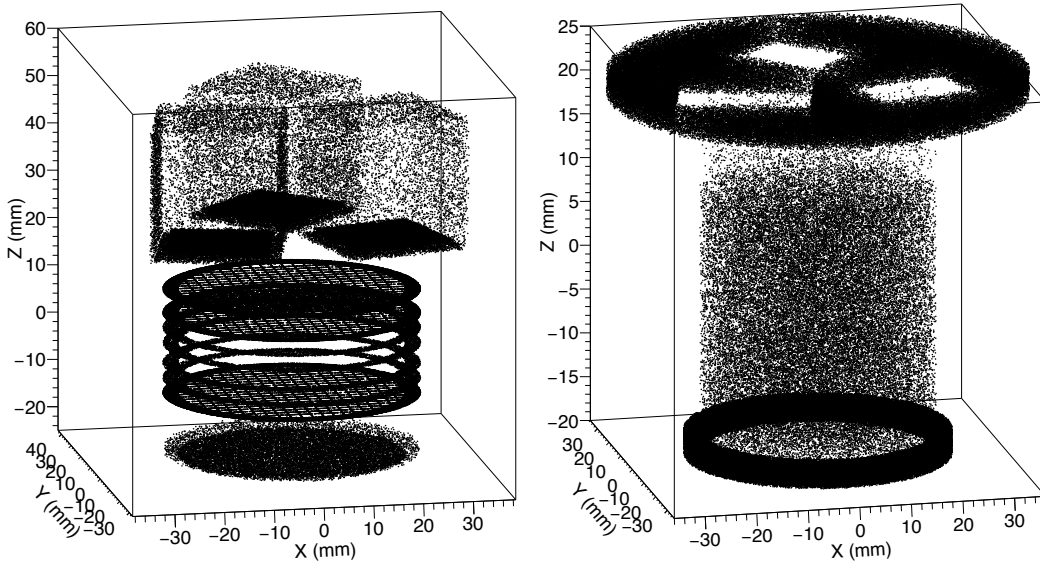


Figure 6.7: The BACCARAT TPC model broken into the PMTs, grids and FSRs (left) and the LXe, GXe, and PTFE sockets (right).

The walls of the TPC are modeled as a flush cylinder, composed of stacked PTFE and stainless steel rings (of accurate thickness). The floor of the TPC is composed of a bottom PMT window and photocathode surrounded by a PTFE socket ring, and the ceiling is composed of a PTFE socket (with windows cut out) and top PMT faces. Fig. 6.7 breaks the model into two parts for visualization of key components.

In addition to the steel FSRs, realistic mesh grids are created by taking the union of iteratively-generated thin wires, all rotated and constrained to the inner diameter of the

TPC. However, since the mesh is square and not hexagonal, the wire pitch is taken to be the average of the smallest (2 mm) and largest (2.31 mm) distances across a true hexagonal cell. As will be shown, simulations were run with alternate wire pitches, to little effect. A LXe cylinder is defined from the bottom PMT to 3 mm above the gate; a GXe cylinder is created from the liquid surface to the top PMTs.

6.3.1 Estimating our S1 Efficiency

To quantify the LCE for events generated in the vicinity of our source, we run a photon bomb simulation by isotropically generating 5000 photons per 0.25 mm^2 pixel in a 1 mm-tall cylinder, extending just above and just below the z coordinate of our fused silica source in the drift region. We then track the destination of each photon generated from each pixel (or photon bomb), and consider a photon “detected” when it hits a PMT (we account for PMT efficiency later). We then lump photon bombs into r^2 bins and calculate the average LCE, or the fraction of photons which hit a PMT, for each bin.

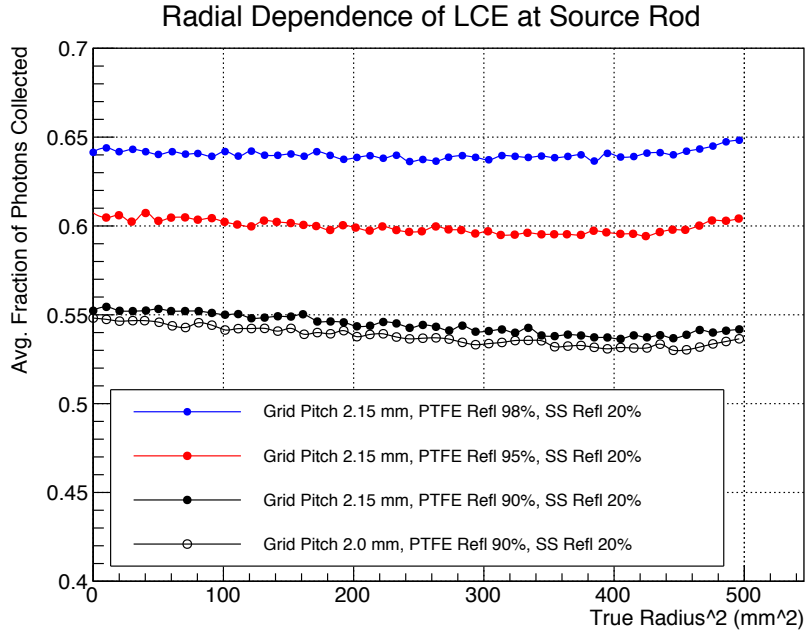


Figure 6.8: The r^2 dependence of the LCE for various PTFE reflectivities and grid pitches.

Fig. 6.8 shows the results for a number of material parameters. It is known that the

VUV reflectance of stainless steel is quite low [132], so we use a 20% reflectivity for all optical surfaces in contact with steel. Measurements have shown that PTFE is highly reflective in LXe, with some variation [167]; therefore, we vary the reflectivity from 90-98%. Notably, high PTFE reflectance results in a 1% upturn of the LCE near the walls; this effect goes away with the reflectivity at 90%. PTFE in contact with GXe is set to a reduced 80% reflectivity. With a conservative PTFE reflectance, we also performed a simulation with a worst-case grid pitch of 2 mm, which has a noticeable but tiny effect on the LCE.

From these LCE simulations, we can estimate the overall S1 detection efficiency g_1 using

$$g_1 = \varepsilon \cdot \text{LCE} (1 + \text{DPE}) \quad (6.3.1)$$

where ε is the quantum efficiency of the PMT and DPE is the well-known probability for double photoelectron emission of photocathodes at VUV wavelengths. With $\varepsilon \approx 0.3$ [114, 115] and $\text{DPE} \approx 0.2$ [96], we get $g_1 \approx 0.19$ phe/(S1 photon) at $r = 0$; this value is reasonable when compared with other small Xe TPCs [54, 222].

6.3.2 Optimizing Position Reconstruction

Photon bomb simulations are also useful for studying the gas gap, where S2 light is produced and distributed amongst the PMTs. Since we have very few PMTs, we have very few pixels with which to perform position reconstruction. Thus, it is very important that we determine the viability of position reconstruction algorithms and maximize our position resolution.

We run a simulation as described in the previous section, but with photons generated from a thin cylinder in the middle of the 2 mm gas gap. For each photon bomb, we tabulate the number of photons that hit each top PMT to generate a “hitmap”. We then use a simple centroid (a.k.a. center of gravity, or CoG) algorithm to reconstruct the position of the photon bomb from a weighted average:

$$x_c = \sum_i \frac{n_i x_i}{n_{\text{top}}}, \quad y_c = \sum_i \frac{n_i y_i}{n_{\text{top}}} \quad (6.3.2)$$

Here, (x_i, y_i) is the coordinate of the i th PMT pixel and n_{top} is the total number of hits in the top array. This algorithm is prolific and has been applied in γ imaging [161, 171], charge

readouts in electron drift chambers [140], and photosensor arrays using SiPMs or PMTs [178, 215].

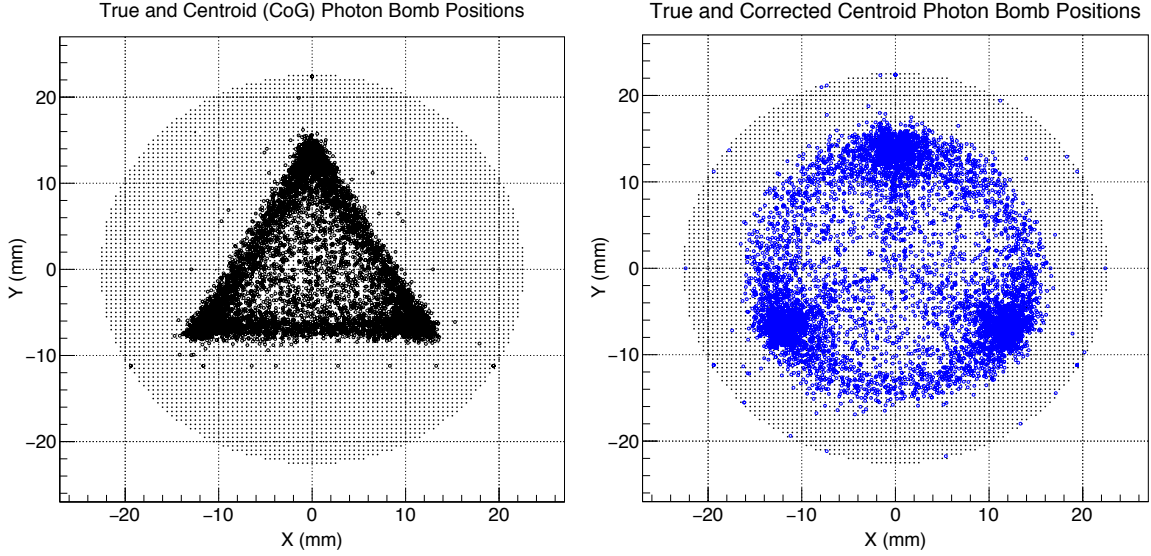


Figure 6.9: Photon bomb positions reconstructed using CoG (left) and corrected CoG (right).

From Fig. 6.9, we see that the centroid algorithm causes significant warping of the photon bomb positions. The resulting xy distribution is triangular, mirroring the layout of the top PMT array. There is also a radial “shrinking”, which is typical in center-of-gravity algorithms due to the finite extent of the distribution [25]. The optical warping is made even more significant by our having only 3 large pixels, since the position resolution depends on the pixel spacing [227].

We can implement a geometric correction to partially account for asymmetric warping by transforming into a sub-angle of the triangular distribution ϕ' and correcting the radius as a function of this angle. The angle ϕ' is calculated using the uncorrected ϕ by

$$\phi'(\phi) = \left| \phi - \frac{\pi}{2} - \text{int} \left(\frac{\phi - \pi/2}{\theta} \right) \theta \right|$$

where $\theta = 2\pi/3$ is the angle spanned by a triangular side. The radial correction factor to push an event at radius r back out to PMT radius R is

$$\alpha = \frac{R}{r} = \sqrt{3} \sin \phi' + \cos \phi' \quad (6.3.3)$$

From Fig. 6.9, we see that this corrected centroid (CC) algorithm gives a more geometrically reasonable distribution, but has a strong angular dependence since the warping is not simply a radial effect. While this asymmetry is not ideal, it does reduce leakage of events from the periphery into a central fiducial volume.

There are a variety of other more refined position reconstruction methods (e.g. truncated center of gravity TCoG, raised-to-the-power RTP, maximum likelihood, weighted least squares) [178, 215] that could be used to improve results. However, given that we have such few pixels for position reconstruction, such efforts have diminishing returns. Linearity may improve at the expense of resolution in some cases [171]. We therefore focus on simple, computationally fast corrections that optimize our background leakage and fiducialization.

Another method which falls into this category utilizes our S2 photon bombs in a straightforward manner; we can generate a Monte Carlo look-up table (LUT), which provides the mapping between our uniform grid of true photon bomb vertices and the optically warped positions computed by CoG. Since the S2 signal is what we measure in experiment, we start by calculating the CoG positions for each photon bomb, then perform a 2-dimensional IDW interpolation (see Sec. 3.6.1.2) with the LUT to extract a corrected position. This procedure is performed using various numbers of nearest neighbors (NN) in the IDW interpolation, in order to optimize the algorithm. Results are shown in Fig. 6.10.

A comparison between the centroid, CC and LUT methods is shown in Fig. 6.11 for high-statistics and low-statistics simulations. The leakage fraction as a function of r^2 is defined as the number of events with true position $> r^2$ that are reconstructed $< r^2$. For the simulation where each photon bomb produces 5000 photons (which is a rather small S2 after factoring in photon detection efficiency), the statistical error is low enough that we can clearly identify systematics. It is clear that CC reduces the leakage fraction at all radii compared to the original CoG. LUT interpolation has worse leakage below a characteristic r^2 , but much better leakage as the fiducial is expanded beyond this “clumping” point. It is interesting to note that increasing the number of NN in the LUT interpolation gives better leakage at lower radii, but only because the events become more clumped at large r^2 (see

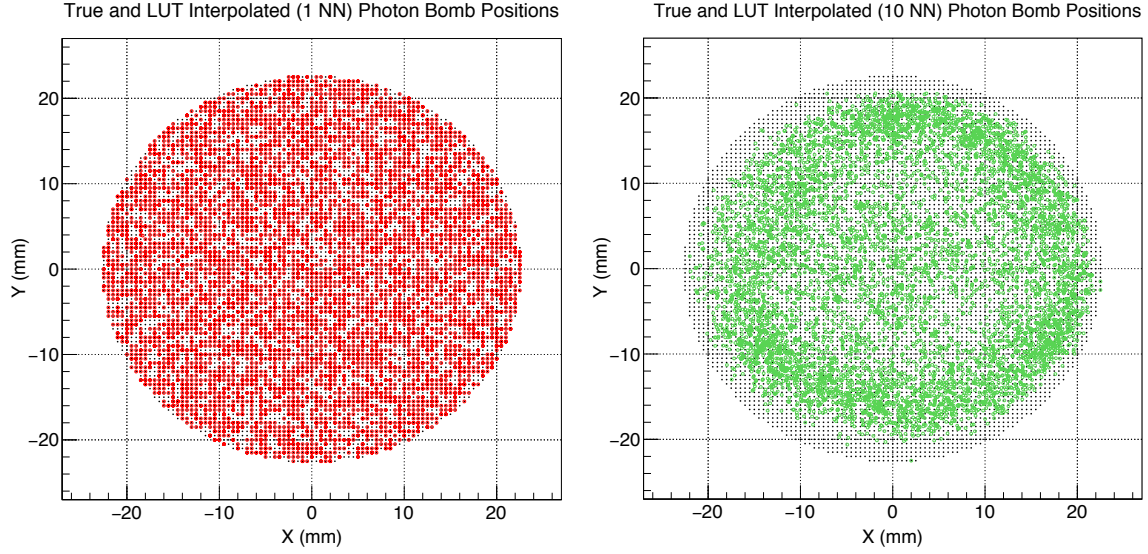


Figure 6.10: LUT-interpolated positions calculated using different numbers of NN.

Fig. 6.10).

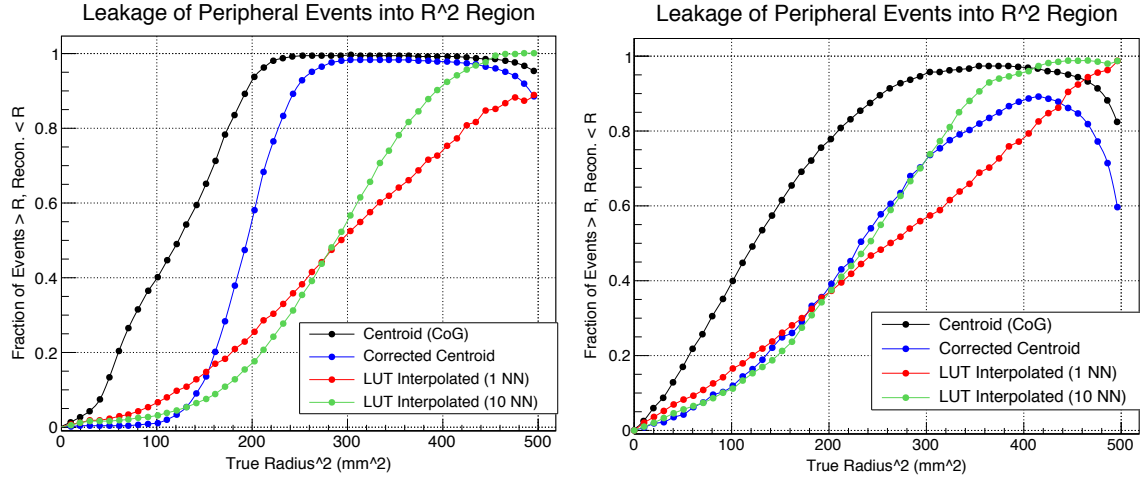


Figure 6.11: Leakage of events $> r^2$ into a fiducial volume at r^2 for a 5000 photon-per-bomb simulation (left) and 500 photon-per-bomb simulation (right).

For the lower-statistics simulation, where 500 photons are released in each photon bomb, leakage is worse for all algorithms at low r^2 . Statistical errors are large for this simulation, which is why the leakage curves are much more linear and systematic differences between

the CC and LUT algorithms are nearly negligible. This means that for a worst-case S2 size, where the position uncertainty is very high, CC or LUT algorithms have similar leakage.

It is important to look not only at the leakage, but also at the position reconstruction residuals. One can always systematically shove all events into the periphery, but this lowers our detection efficiency when a fiducial cut is implemented. The radial dependence of the residuals is shown for our algorithms in Fig. 6.12.

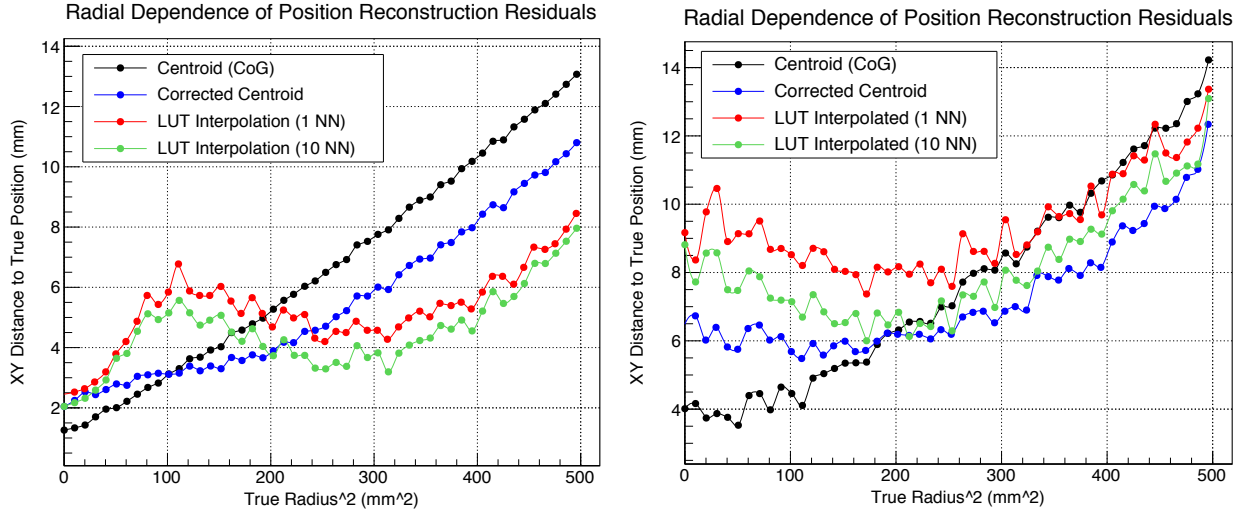


Figure 6.12: Position reconstruction residuals for a 5000 photon-per-bomb simulation (left) and 500 photon-per-bomb simulation (right).

The LUT interpolation clearly benefits from local MC information, as the residuals are better at large radii. However, the results are worse near the center of the detector, where systematic uncertainties in the IDW interpolation actually lead to worse residuals than the CoG algorithms. The CoG residuals are sensible, since the statistical error in the S2 reconstruction scales as $\sigma \sim 1/\sqrt{n_{\text{hits}}} \sim 1/\sqrt{S2}$ [25], and the S2 size decreases with radius.

It should be noted that the residual is only a proxy for the position reconstruction error when the statistical uncertainties on the S2 are subdominant. Small S2 signals result in a large statistical uncertainty which will become a significant component of the error. Furthermore, position resolution will show a strong dependence on the S2 size in real data, and this variation will make it difficult to realistically implement a purely MC-based LUT

interpolation. However, it appears from this study that position reconstruction using one of these corrected algorithms is feasible, at least for fiducializing the central source region.

6.4 Electric Field Simulations with COMSOL

A primary goal of this thesis is to disentangle the various issues which plague the periphery of Xe detectors. In an effort to do just this, it is important that we characterize the electric field profile to avoid large systematic uncertainties in the Xe response.

Shown in this section are results for 3D electrostatic simulations of the DAX TPC using COMSOL Multiphysics[®]. For simplicity, we limit the discussion to an optimal configuration for maintaining uniform fields at the maximum grid voltages reasonably achievable given our tight detector spacing. As such, this simulation serves as a worst-case scenario in terms of extraction field leakage, but with the caveat that the COMSOL geometry was simplified as discussed in the next section.

6.4.1 3D Meshing of a Simplified TPC Model

To design the detector components and assess any conflicts with mechanical constraints, a detailed model of the TPC assembly is built in the Autodesk Inventor design software. In this environment, all TPC components are assembled and placed inside of a stainless steel inner can with a thin PTFE liner, resulting in a realistic representation of the Xe space. Furthermore, this model can be exported into a STEP (.stp) file format for importing into COMSOL via the CAD Import module. After import into COMSOL, the Xe space within the steel can is “filled” with LXe and GXe by projecting cylindrical volumes from a plane at the desired liquid level and forming a union with the other domains of the model in the Finalization step of the Geometry sequence.

The greatest challenge with performing a COMSOL simulation is generating the appropriate mesh for the model. COMSOL uses the finite element method (FEM) to approximate solutions to partial differential equations (PDEs) for complex geometries, which involves

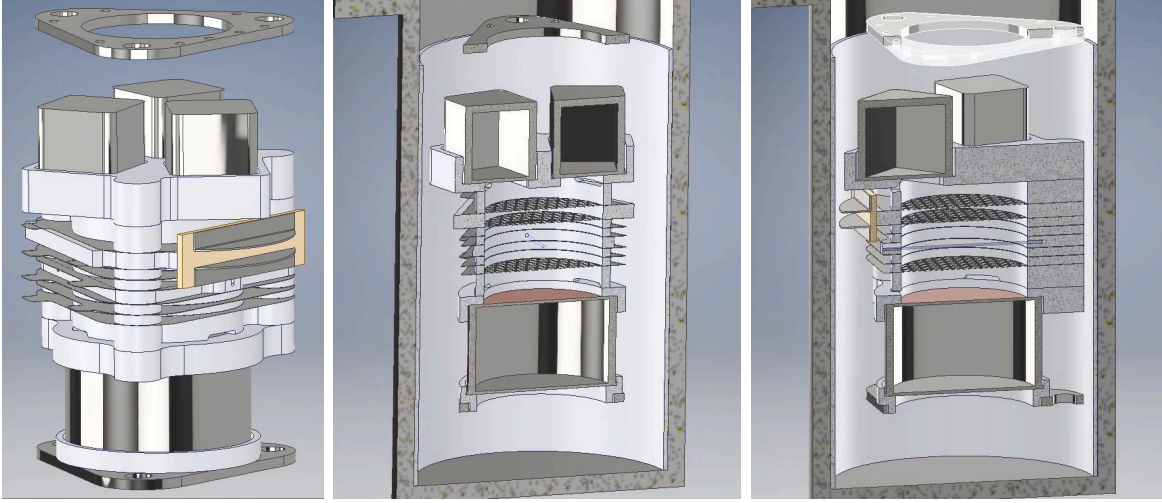


Figure 6.13: (Left) External view of the TPC model in Inventor. (Center) Cross section slicing perpendicular to source rod, with surrounding inner can and PTFE insulation. (Right) Cross section slicing along source rod axis.

breaking the geometry into finite polyhedral elements (whose corner points are known as “nodes”) and solving a system of simultaneous equations constructed from basis interpolation functions [79]. Such a tessellation is called a “mesh”.

Geometries with finer features require finer meshing, since the interpolation across large elements would lead to a poor local approximation of the true solution of the PDE. However, finer meshing comes at the cost of greater computation time and memory consumption. The DAX TPC model necessitates an extremely fine mesh for some components, particularly the $50\text{ }\mu\text{m}$ mesh grids, and COMSOL requires an enormous amount of resources for meshing and solving such a model. Therefore, we take great care to simplify the fine details of our CAD model before importing into COMSOL, as tiny features (especially those in close contact) may result in non-convergence of the mesh. A separate copy of the Inventor model is simplified with a removal of threaded screws, small holes, and other tiny enclosed volumes; vacancies are filled with appropriate materials to maintain a realistic electrostatics model. It should be noted that our TPC model also does not include smaller components outside the active region, such as the HV connectors, cables, and resistor chain.

To optimize the simulation and reduce the memory consumption to our computational capacity, domains were meshed in independent groups (i.e. finer parts and regions of interest were more finely meshed than others). Once the 3D meshes are generated by COMSOL, the material of each domain may be specified and customized. Voltages on the bodies of the PMTs, grids, field-shaping rings (FSRs), and level meter capacitor plates are then set based on the desired configuration. After setting all material and voltage parameters (given in the table below), an electrostatic simulation is performed using the full mesh. Fig. 6.14 shows an external field profile of the 3D model, which we break down in more detail in the following sections.

Component	COMSOL Material	Permittivity, ϵ	Voltage
LXe	Custom	1.9	N/A
GXe	Custom	1	N/A
PTFE/PEEK	Custom	2.1	N/A
Fused Silica	Custom	3.7	N/A
Anode	Steel	N/A	−800 V
Gate	Steel	N/A	−4.5 kV
FSRs 1-4	Steel	N/A	−5.7, −5.4, −5.1, −4.8 kV
Cathode	Steel	N/A	−6 kV
PMTs	Steel	N/A	−800 V

6.4.2 Drift Field Profile

Of particular interest is the electric field profile in the drift region, since this determines the light and charge yields of our sources and may cause variation in the electron drift trajectories. One way to inspect the electric fields in the drift region is to make a cut plane that slices through the 3D solution in COMSOL and plot the directionality and magnitude of the fields. Such a plot is shown in the top of Fig. 6.15.

The results show quite a uniform field in the middle of the detector, specifically in the

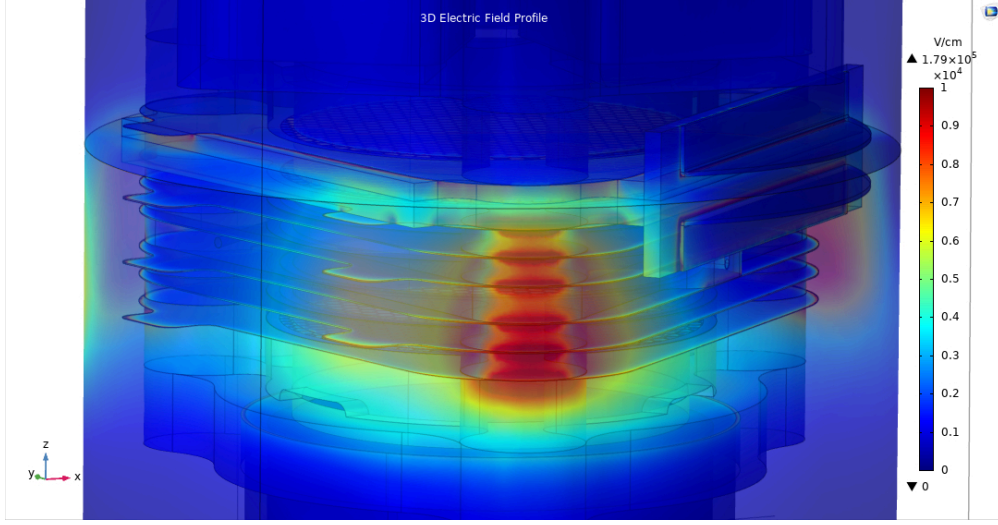


Figure 6.14: A 3D field profile from an electrostatic simulation of the TPC.

region of interest between the source rod and the gate grid. There are observable “field fringing” effects in the periphery due to leakage of the high field extraction region into the drift region, however such variation is minimized with the recessing of grids and FSRs into the insulating PTFE walls.

A plot of the electric field magnitude as a function of z coordinate is also made using a cut line through the model at $r = 0$. This shows the uniformity of the drift field, with some variation near the cathode and gate grid wires and in the local neighborhood of the fused silica rod. As expected, the field is discontinuous at the rod where the dielectric constant suddenly changes. What we wish to characterize are the fields in the LXe just above the surface of the rod, however the COMSOL simulation has limited mesh size and cannot compute fields down to the sub- μm level in our large geometry. Assuming a smooth field profile at the interface between two neutral dielectrics, we may assert that the observed field variation is due to the geometric curvature of the rod. In this case, the 25% upper fluctuation of the field at the rod surface may be taken as a measure of our field uncertainty at the interaction site of our source.

Given the axial asymmetry of the TPC, it is also important to examine the xy profile of the fields. By making cut planes at various heights, we may examine z slices of the drift

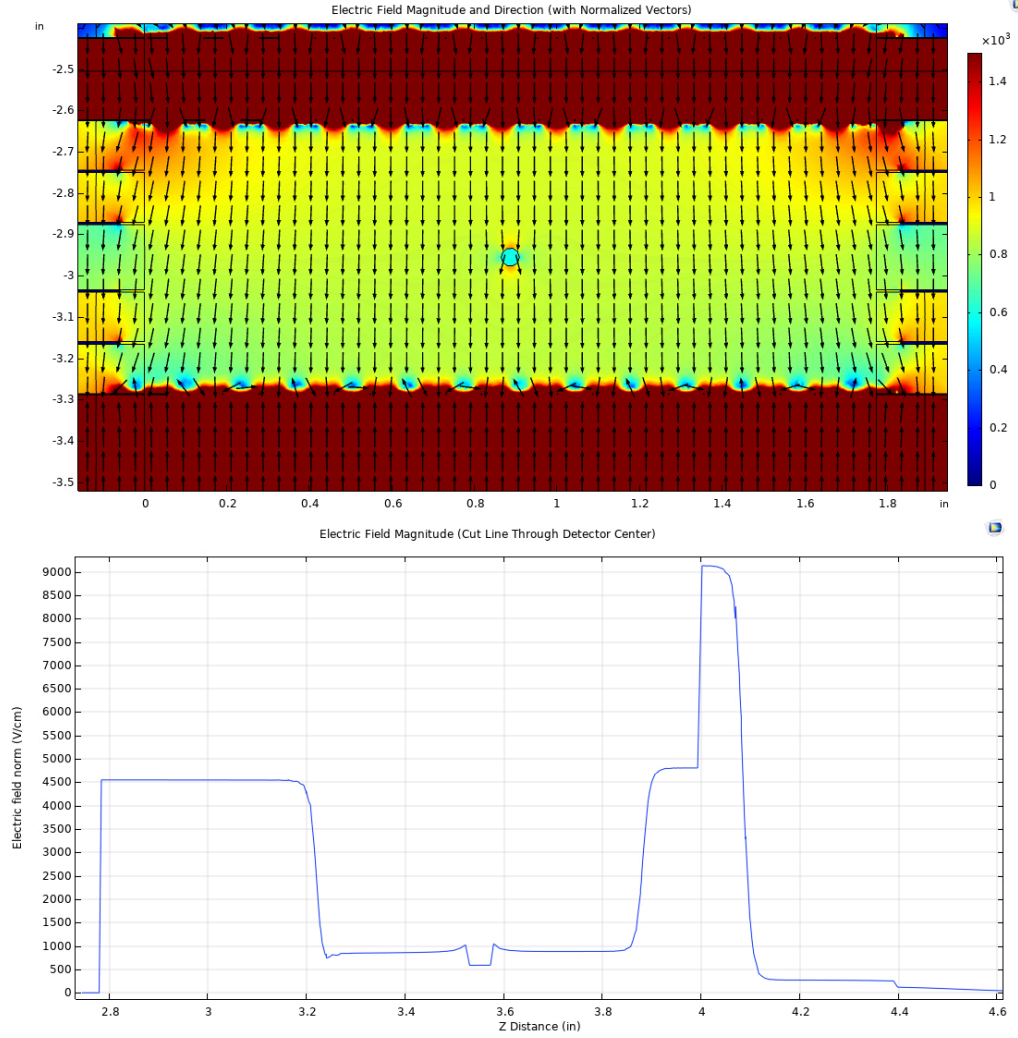


Figure 6.15: (Top) 2D plane cut on a COMSOL simulation, with colormap representing electric field magnitude in V/cm and the arrows indicating direction. (Bottom) Field z profile using a cut line at $r = 0$, showing fields in all regions of the TPC.

region. In Fig. 6.16, we see the fields are quite uniform outside the volume of the source rod. As the z plane is shifted up, the leakage field in the periphery is more prominent, however this appears to minimally (and symmetrically) affect our centralized source as the electrons approach the liquid surface.

The xy plots also support the origin of the leakage fields. The top plot shows a highly uniform field between the field shaping rings (bright yellow), whereas the bottom plot at

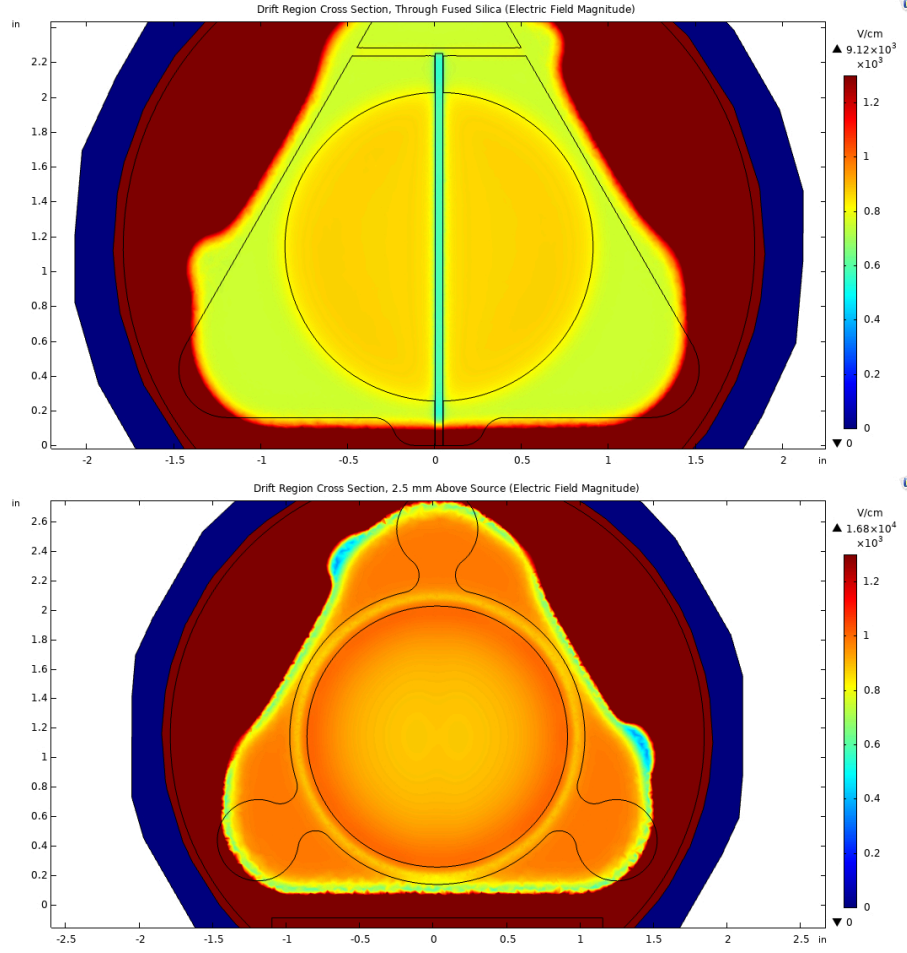


Figure 6.16: Field xy profiles from a cut plane through the center of the drift region (top) and 2.5 mm above the source rod (bottom).

higher z shows much lower fields on the edges of the field rings and higher fields where insulation from the extraction region is reduced. Note also that the contact tabs extending from the sides of the grids are resolved as a feature in the field profile.

6.4.3 Extraction Region

Studying the extraction region is of great importance to our charge yield measurement, since the S2 signal is highly sensitive to detector parameters. We care about maximizing our electron extraction and minimizing non-uniformities to produce a stable S2 signal.

The S2 signal depends on numerous detector parameters, so it is worth taking time to disentangle them. The S2 may be broken down into

$$\text{S2} = g_2 N_e = \eta \psi N_e \quad (6.4.1)$$

where η is the efficiency of extracting the N_e ionization electrons produced at the interaction site and ψ is the single electron size in photons per extracted electron.

This separates the S2 yield into two important components which differently depend on the extraction field. The extraction efficiency is a function of the extraction field, and most recently have been measured by the PIXeY detector [93] to be

$$\eta = -0.03754 E_{\text{liq}}^2 + 0.52660 E_{\text{liq}} - 0.84645 \quad (6.4.2)$$

where E_{liq} is the extraction field in the liquid phase (between gate and surface) in kV/cm.

The other component, the measured photons per extracted electron, depends on both the electroluminescence yield y and the light collection in the extraction region g_1^{gas} . The electroluminescence light produced has a linear dependence on the gas gap size, however the so-called “gas gain” also depends on the electric field and gas pressure. The overall single electron size is then given by

$$\psi = g_1^{\text{gas}} y = g_1^{\text{gas}} (\alpha E_g - \beta p - \gamma) h \quad (6.4.3)$$

where E_g is the electric field in the gas phase, p is the pressure in bar, h is the gas gap height in cm, and the other constants are empirically derived [75].

Lastly, to understand the relationship between E_{liq} and E_g , we frame the extraction region as a capacitor problem. Taking a parallel plate capacitor with a uniform field and inserting two different dielectrics (of different heights) in series, a simple calculation yields

$$E_g = \frac{\epsilon_l}{\epsilon_g} E_{\text{liq}} = \frac{\epsilon_l}{\epsilon_g} \left[\frac{V_{ga}}{d_{ga} + \left(\frac{\epsilon_l}{\epsilon_g} - 1 \right) h} \right] \quad (6.4.4)$$

where ϵ gives the corresponding dielectric constant, V_{ga} is the voltage across the gate-anode gap, and d_{ga} is the gate-anode distance. We can see from Fig. 6.17 that the fields in the liquid and gas phase indeed differ by about a factor of $\epsilon_l/\epsilon_g \approx 1.9$.

What is noteworthy about these formulae is that there is not an obvious set of ideal detector parameters, since there are competing effects. For example, a smaller gas gap increases the extraction field but decreases the gas gain; it is non-trivial to optimize both. However, operational constraints typically keep the pressure somewhere in the range $1.5 < p < 2$, which means that most of the variation in the S2 size comes from the gas gap size (i.e. liquid level) and the applied extraction field.

For our measurement, we desire sensitivity to extremely small charge signals and therefore wish to maximize our extraction efficiency. Furthermore, raising the liquid level increases the separation between the extraction surface and the source rod, allowing better discrimination from surface backgrounds and spurious electron emission [216, 230]. Therefore, we expect to operate with the liquid level at least 2.5 mm above the gate, or with a gas gap of at most 2.5 mm. Given that the light in our TPC is concentrated in just 4 PMTs, there is high likelihood of saturation even for relatively small signals, and therefore it is reasonable to sacrifice gas gain for a higher extraction efficiency.

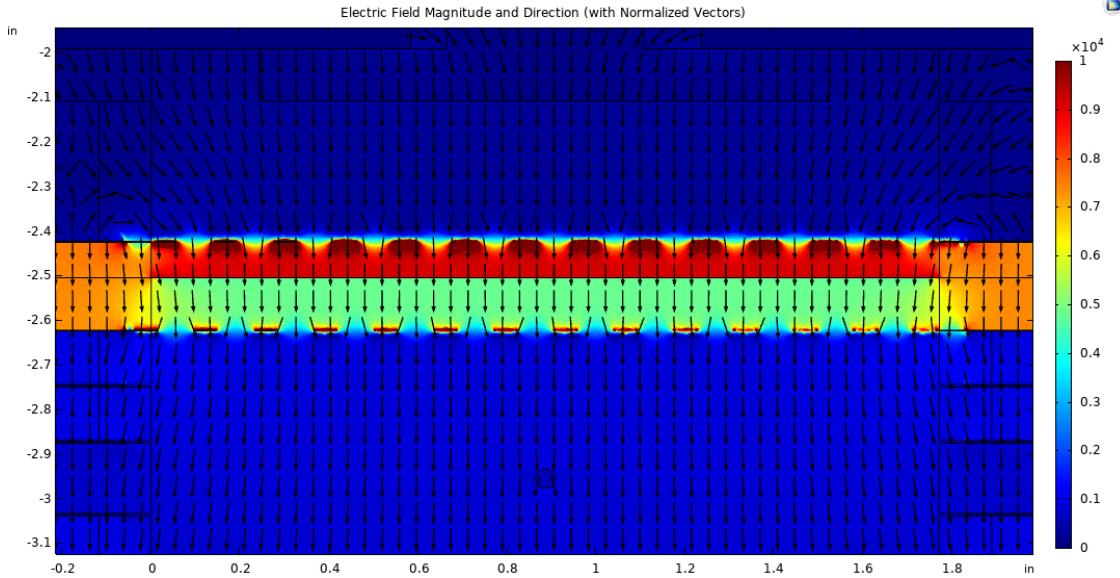


Figure 6.17: A 2D cross section of the extraction region in COMSOL.

From Fig. 6.17, we see that for a 2 mm gas gap (resulting in higher E_g) our extraction fields remain quite uniform even out to large radii. This implies that the stability of our S2

signal will almost be exclusively tied to the stability of our liquid level, given that we can achieve the desired gate and anode voltages.

Note that this plot gives a worst-case scenario for “electron transparency”, as this cut plane slices along the axis of the hexagonal mesh wires; in alternate cut planes, this visibly improves. Looking at an xy cut plane through the center of the gas gap (Fig. 6.18), we can actually resolve the mesh pattern in the field profile. The extraction fields in the gas phase are quite axially symmetric, however, which is encouraging for uniform extraction and ideal position reconstruction using S2 signals.

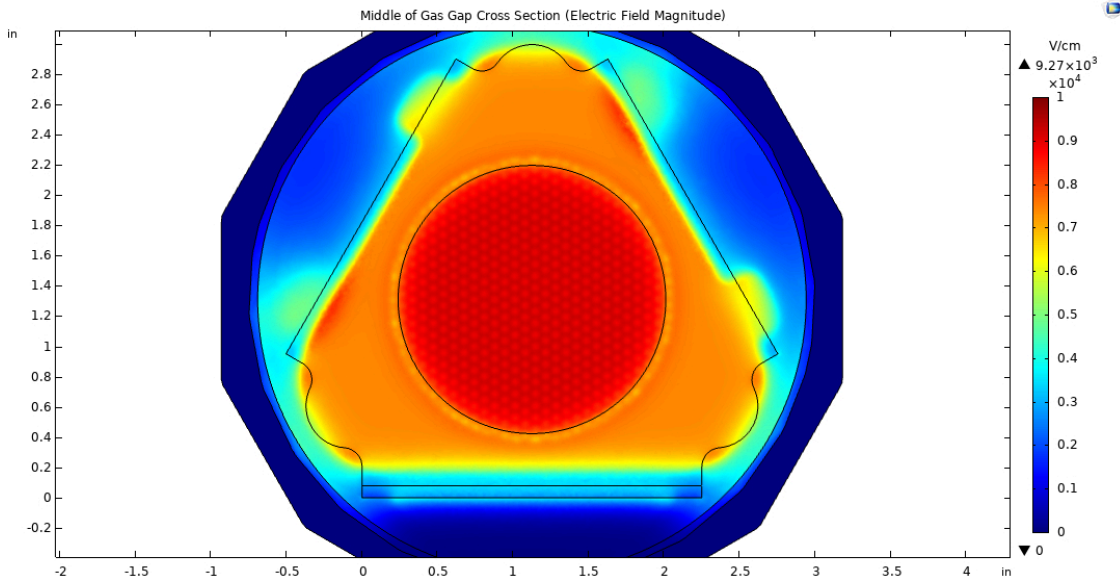


Figure 6.18: An xy cross section of the center of the gas gap in the extraction region.

6.4.4 Top and Bottom Reverse Field Regions

A major factor determining the high voltage configuration of our grids is the field profile in the non-drift regions, or the reverse field regions (RFRs). The region between the bottom PMT and cathode (bottom RFR) is a large volume of liquid that acts as a target for background events; to prevent electrons from drifting up from this region, we ensure that the field here is reversed to drift electrons downward. Similarly, in the region between the anode and the

top PMTs (top RFR), we ensure that the fields in the gas region drift electrons away from the anode so they do not produce S2 light in the gas gap.

Since our PMTs operate only in a small voltage range ($\approx 800\text{--}1000\text{ V}$), we are constrained in the reverse fields we can produce. To create the RFRs, we negatively bias our anode grid to the top PMT voltage ($\approx -800\text{ V}$), which creates a small reverse field in the top RFR (see Fig. 6.19). Gas events created in this region have highly characteristic signals, namely S1 and S2 signals which are nearly inseparable in time, and can thus be easily rejected.

This anode voltage then fixes the rest of the HV circuit. The gate is coupled to the FSRs and cathode through a resistor chain, and the gate and cathode are set based on the desired extraction and drift fields. For this specific simulation, the gate is set to -4.8 kV and the cathode is set to -6 kV , pushing the boundaries of our high voltage capabilities in DAX. Note that such a cathode voltage automatically produces a strong reverse field in the bottom RFR, since the bottom PMT is set to a maximum magnitude of 1 kV .

6.4.5 High Field Regions

COMSOL simulations are useful in another capacity: the identification of potential high voltages issues. The spacing of the DAX detector is very tight, resulting in high voltage delivery through low-profile cabling and connections. The close proximity of such components is a recipe for electrical sparking in our high voltage setup.

It is well-known that conductors with sharp edges produce local high field regions, which may result in breakdown of the dielectric and the formation of a conductive ionization channel between surfaces (“sparking”) [156, 183]. This requires sufficient insulation to protect components, especially active electronics such as the PMTs and level meter capacitors.

We have taken some measures in the detector design to maximize electric field uniformity. The grids and FSRs were specifically constructed to extend outside the PTFE spacers to move the high-field edges into the surrounding LXe skin. However, this moves these edges closer to the conductive steel can. Therefore, an additional PTFE film lines the steel can to provide a buffer between the high voltage components and the steel wall. From Fig. 6.20,

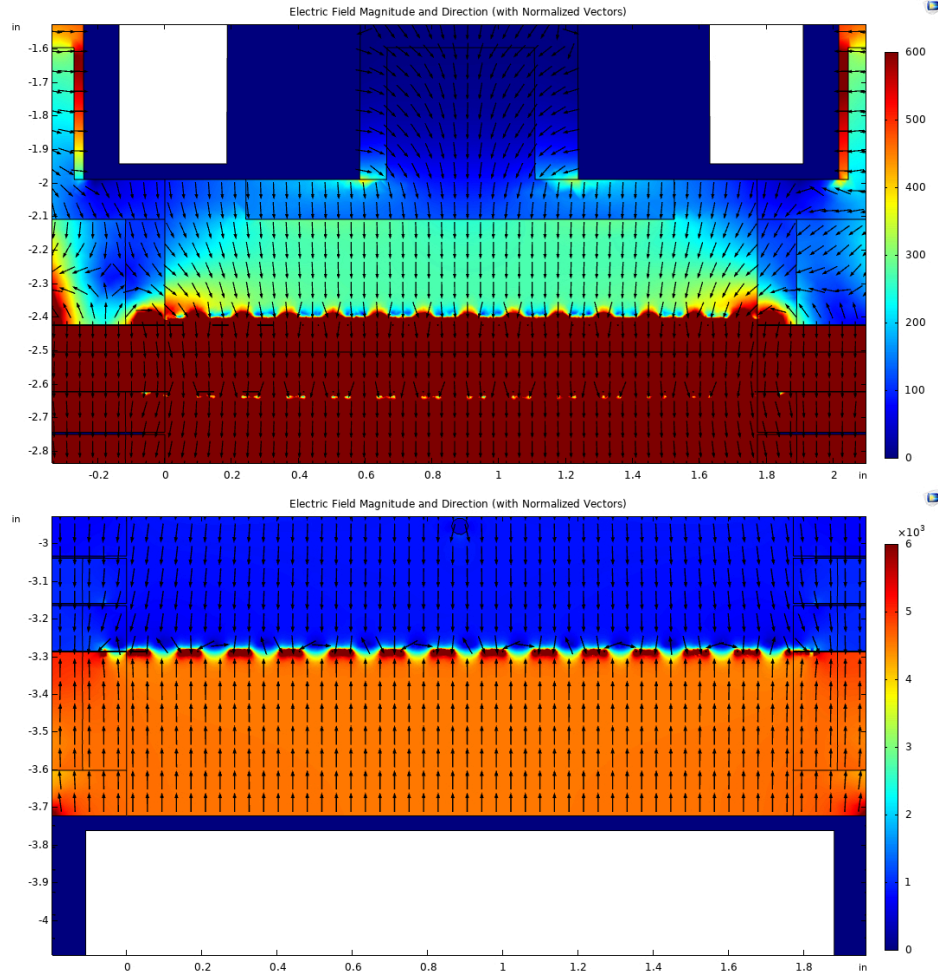


Figure 6.19: The field profile of the top RFR and bottom RFR.

we see that the PTFE components indeed act as excellent high voltage insulators. However, in the surrounding LXe, particularly at the corners of the TPC and at the level meter, HV concerns persist and are the limiting factor on our applied grid voltages.

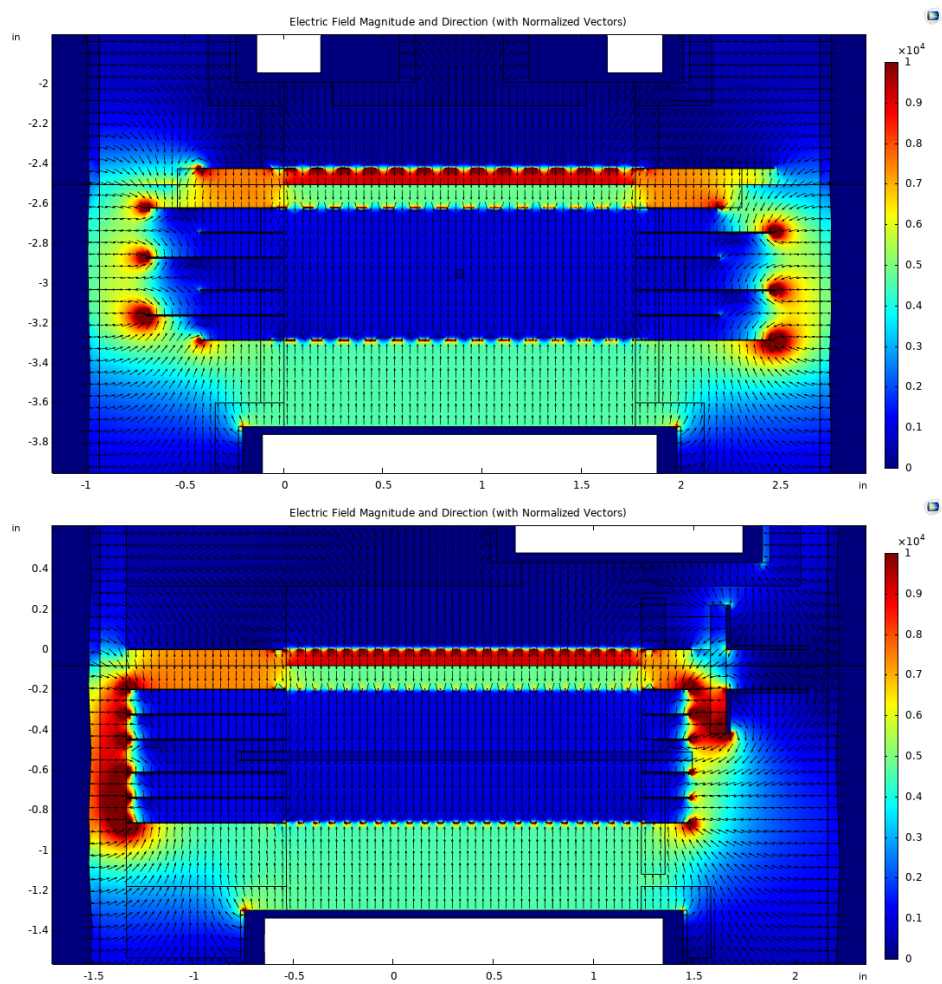


Figure 6.20: Multiple cross section views of high field regions in the TPC.

Chapter 7

A Direct Measurement of ^{206}Pb Yields in Liquid Xenon

The ultimate purpose of our extensive simulation work is to optimize our detector design to make accurate nuclear recoil measurements. The new and improved DAX TPC was assembled with these details in mind, as we hope to separate the various detector effects which hinder characterization of backgrounds in the periphery of Xe detectors.

In this chapter, we present a measurement of LXe response to ^{206}Pb recoils. We will summarize the code framework used for our data analysis, as well as our latest technique for creating localized sources. This technique is used to employ not only a ^{206}Pb source, but also an internal ER source of various energies (^{109}Cd) in order to perform a precise, local detector response calibration. This allows us to present light and charge yields for ^{206}Pb recoil ions.

7.1 A Localized Source Deposition Procedure

To create a localized source on a fused silica rod, we implement a new procedure for functionalizing the surface using an adhesion promoter. This procedure is different from the one discussed in Sec. [5.4](#), since we are now both minimizing the thickness of the source layer

and adding a masking procedure to constrain the active surface area.

To optimize the optics and purity of our substrate, we use rods stretched from UV-grade Suprasil fused silica, custom-made by NJPB Glass. The rods used for these measurements are ≈ 1.12 mm in diameter, and are carefully cut to a length of 5.8 cm. This length ensures that the source is centered in the active region when the rod is centered in its PTFE holder spacer. An obvious but important consideration is to ensure that the orientation of the source is well-defined at installation, since the mono-molecular source layer is not visible on the rod after deposition. The rods are therefore beveled at an end so that the source may be installed in the TPC with the source pointed upward in the drift region.

Our goal is to achieve a source localized to ≈ 1 mm² surface area at the center of the rod, spanning $< 180^\circ$. If the source layer were to form a ring, any events occurring in the LXe below the rod would have compromised charge collection due to the directionality of the drift field and potentially wash out our S2 signal. Limiting the angle subtended by the source limits the contribution of such events, provided the source is placed with proper orientation. To achieve this, a metal jig with angled edges clamps down on the rod to expose only the central surface during source deposition.

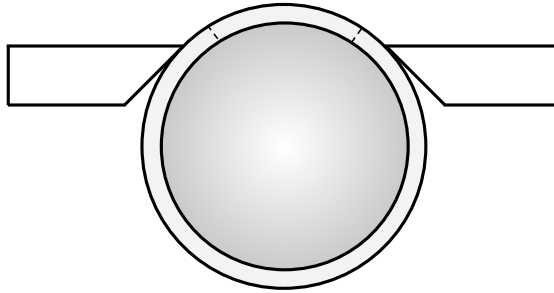


Figure 7.1: Fused silica rod being masked with PTFE tape under the angled jig edges.

While the jig masks the rod in one direction, it does not prevent the source solution from running along the hydrophilic fused silica surface. Furthermore, the acidic HCl source solution tends to create undesirable side reactions when in direct contact with metal. Several different masking techniques were attempted to address these issues. One method involves immersing the rod-jig assembly in melted wax after preparation, however this complicates the

deposition chemistry, since removal of the wax requires a combination of re-melting the wax and solvent application that may compromise the deposited source layer. We ultimately use PTFE tape to mask the rod and jig, as this material is clean, hydrophobic, easy to manipulate, and soft enough to be cut away.



Figure 7.2: (Left) An example fused silica rod with a beveled end. (Right) The metal jig clamping down on a masked fused silica rod before source deposition.

The last remaining question is how to ensure we form a mono-molecular layer while maintaining a reasonable source activity. The liquid sources we use come as a chloride, e.g. PoCl_4 , in 2 Molar (M) hydrochloric acid (HCl). When deposited as a liquid and dried, the evaporation of water leaves behind a sub-nm layer of molecules. In fact, the source is dilute enough that many layers of the source can be deposited and dried without fear of forming a thick layer. The limiting factor in our deposition is the adhesion promoter (AP) TMS-ED3A, which has large molecules which form a glassy layer when dried. However, we can dilute the AP enough to minimize the thickness of such a layer.

The mass of AP needed to give a roughly mono-molecular layer can be approximated for a surface area ℓw , thickness h , and density $\rho_g = 2.5$ (that of glass):

$$m_{\text{AP}} \approx \ell w h \rho_g$$

If we dilute an initial volume of AP liquid $V_{\text{AP},i}$ of density ρ_{AP} using a volume of water $V_{w,i}$, we obtain a liquid volume $V_{\text{liq},i}$. The *deposited* mass per *deposited* volume is then given by

$$\frac{m_{\text{AP}}}{V_{\text{liq}}} = \frac{m_{\text{AP},i}}{V_{\text{liq},i}} = \frac{\rho_{\text{AP}} V_{\text{AP},i}}{V_{w,i} + V_{\text{AP},i}}$$

Some algebra yields the amount of water needed to dilute $V_{\text{AP},i}$:

$$V_{w,i} = \left(\frac{V_{\text{liq}}}{\ell w h} \frac{\rho_{\text{AP}}}{\rho_g} - 1 \right) V_{\text{AP},i}$$

Suppose that we want to deposit a droplet with volume $V_{\text{liq}} = 1 \mu\text{L}$ (1 mm^3) on the surface of the rod. Taking $V_{\text{AP},i} = 1 \text{ mL}$, $\ell w = 1 \text{ mm}^2$, $h = 1 \text{ nm}$, and $\rho_{\text{AP}} = 1.2 \text{ g/mL}$, we get $V_{w,i} = 5 \times 10^5 \text{ mL}$. This yields a dilution factor of

$$d = \frac{1 \text{ mL}}{1 \text{ mL} + (5 \times 10^5 \text{ mL})} = 2 \times 10^{-6}$$

We achieve this dilution factor by doing a serial dilution, where 1 mL of AP is mixed with 50 mL of deionized (DI) water, then 1 mL of the first dilution is put into 100 mL of DI, then 1 mL of the second dilution is put into 100 mL of DI. This results in a very dilute AP solution with only enough mass per microliter to form the desired mono-molecular layer.

Furthermore, we can estimate how many bonding sites are available to our source ions for such a dilute AP solution. The maximum activity of our source vials is $A = 1 \mu\text{Ci}$, or $3.7 \times 10^4 \text{ Bq}$. Presuming that we deposit at most a tenth of the source vial ($5 \mu\text{L}$ of $50 \mu\text{L}$), we then have

$$N_s = \frac{A \tau}{\ln(2)} f \sim \frac{(3.7 \times 10^4) \tau}{\ln(2)} \cdot \frac{1}{10}$$

Using the half life of ^{210}Po , $\tau = 138 \text{ days}$, we get $N_s = 3 \times 10^{10}$ source atoms. We proposed adding an AP mass of $m_{\text{AP}} = 2.5 \times 10^{-9} \text{ g}$. Using a molar mass of 462 g/mol , we find that this yields $N_{\text{AP}} = 3 \times 10^{12}$ source atoms. In the worst possible scenario, we therefore have 100 AP sites for every Po ion.

We implemented the following procedure to prepare our final sources:

1. In an inflatable glove bag, the liquid source vial is opened and $50 \mu\text{L}$ of 3 M MEMS-grade HCl is added using a Four E $0.5 - 10 \mu\text{L}$ micropipette. The pipette is then used to iteratively rinse down the sides of the vial, fully dissolving and mixing the source.
2. The fused silica rod is prepared with the following sequence of solvents: acetone, isopropanol, hydrogen peroxide, and DI water. The rod is dried after each solvent, with minimal mechanical contact (to avoid surface charging or scratching).

3. The rod is discharged using a Milty Zerostat 3 anti-static gun. This method is also used to discharge the PTFE tape used to mask both the rod and jig.
4. The masked rod is clamped down in the jig. A clean plastic razor is then used to create a small hole at the center of the rod without scratching the fused silica surface.
5. The rod-jig assembly is moved into the glove bag, where the micropipette is used to deposit $0.5\ \mu\text{L}$ of the source onto the exposed fused silica surface.
6. The jig is removed from the bag and placed on a hot plate to bake at 90°C until the source droplet is completely dried.
7. Repeat the previous two steps until the desired source activity is achieved.
8. Immediately after depositing the last source droplet, the jig is moved onto the hot plate. A $1\ \mu\text{L}$ droplet of diluted AP is deposited onto the source, mixing and reacting with the previously deposited source layer.
9. Bake on the hot plate at 90° for ≈ 15 minutes.
10. Carefully remove the rod and its masking materials without mechanically disturbing the source layer. Discharge the rod once again with the anti-static gun to minimize charging and dust accumulation.

The baking process is done to encourage reactivity of the AP with the deposited source, evaporate the water in the layer, and maximize adhesion. The preparation of the sample with various solvents also causes water on the surface to desorb prior to the deposition, which aids in the sticking of the AP. Following the above steps helps us form a uniform glass and maximize the number of source ions bonded to an AP site.

7.2 Source Installation in the New DAX TPC

Multiple runs were done with the dual-phase TPC in order to perform calibrations prior to our ^{206}Pb measurement. For each run, a different source rod is prepared and installed in

the DAX TPC. The rod is suspended in the center of the drift region using a special PTFE spacer, which is machined with vented clearance holes to snugly hold the rod. Shown in Fig. 7.3 is a view of the TPC active region, with the source facing up at the top PMTs (TPMTs).



Figure 7.3: A view of the TPC active region from below, with the source rod installed.

The same cleaning techniques discussed in Sec. 5.4.3 are used when assembling the new TPC. When appropriate, TPC components are cleaned through sonication with acetone and isopropanol, and more sensitive components are wiped down and spot-cleaned. To minimize the exposure of the source rod, it is installed in its PTFE holder just before mounting the bottom PMT (BPMT) and finishing internal cabling.

The TPC before and after mounting in the inner vessel space are shown in Fig. 7.4. Note that two sides of the TPC have level meters mounted, which allows for partial assessment of internal detector tilt and more precise assurance of the liquid level. The third side is used for the high voltage delivery and resistor chain. Also shown is the TPC fully assembled with internal cables connected. The blue zip ties visible are made from ETFE, a low-outgassing plastic similar to PTFE; these are necessary to secure the siphon tube and loose cables to minimize liquid disturbances and provide mechanical stability.

Lastly, efforts were made to minimize angular tilt of the TPC *prior* to sealing up the inner vessel, since leveling the detector during operations is extremely difficult. With the feet of the vessel frame firmly fixed, small 2-dimensional levelers are used to level the gate-to-

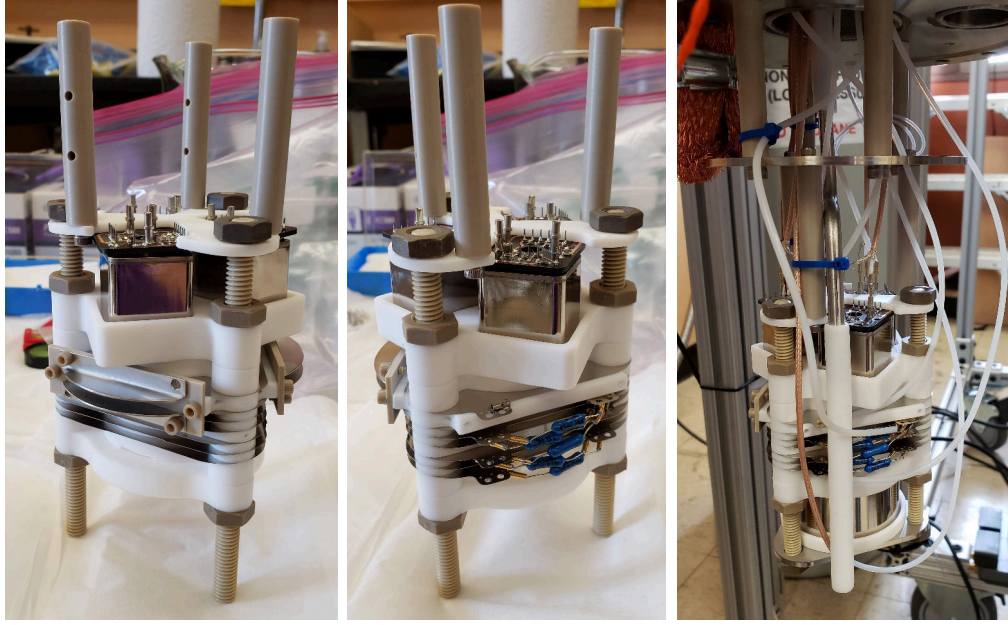


Figure 7.4: (Left) A level meter side view of the partially assembled TPC. (Middle) Side view with resistor chain, grid connections, and source rod holder visible. (Right) TPC hung from the inner vessel ceiling with cabling and BPMT visible.

anode gap relative to the lab floor to within 0.5° of tilt. This corresponds to an uncertainty of ≈ 0.5 mm in the liquid level across the TPC diameter. While this uncertainty is large compared to the ~ 2.5 mm gas gap, consistent electric fields and physical xy localization of the source effectively remove this systematic. If applied voltages and the physical detector configuration are unchanged between runs, we need only be concerned with the uncertainties in the capacitive level meter measurements, which are $\approx 100\mu\text{m}$ when fitting the time-averaged capacitance over the course of a run.

7.3 The ADAX Software Package

The ADAX software package was developed as a comprehensive, self-contained toolset for processing and analyzing data acquired from the DAX detector. This section will provide a summary of the data processing pipeline and signal analysis algorithms.

7.3.1 The Data Processing Chain

For this configuration of the DAX TPC, four PMT signals are fed into an external amplifier. Our amplifier has two output channels for every input channel, so that every PMT signal is amplified independently by both a low gain (LG) and high gain (HG) channel. The signal area gains for the LG and HG outputs (relative to the raw PMT output) are ≈ 4 and ≈ 40 respectively. Therefore, 8 total channels are recorded by the DDC unit for every trigger. This waveform data is then written to a raw binary file format.

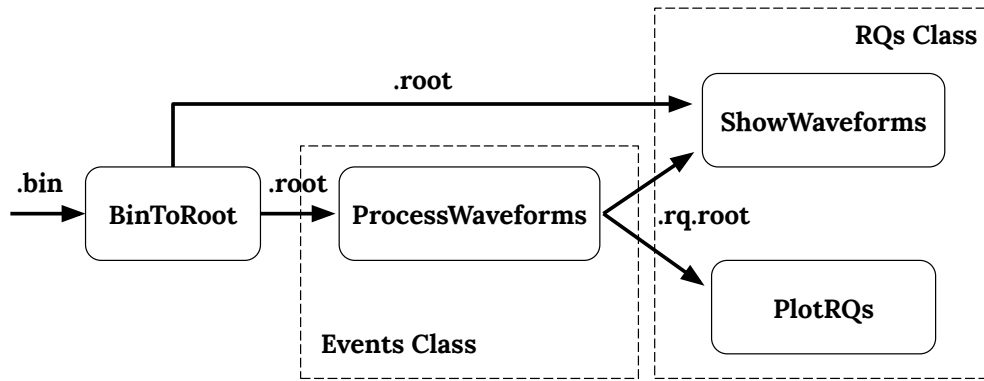


Figure 7.5: A flow diagram of the ADAX processing pipeline.

To make use of this data, the binary file is processed into a ROOT format. ROOT is an object-oriented C++ analysis toolkit developed by CERN for processing and visualizing particle physics data. ROOT files use a compressed binary format which compartmentalizes data according to user-defined classes or data structures. The ROOT library provides data structures that conveniently package data for later retrieval; the tree-like structure (TTree) contains independently-buffered TBranches which are each associated with a class or variable set. Our raw waveform data is stored in such a format by creating an “events” TTree containing separate branches for each recorded DDC channel. The branches contains waveform arrays for each entry, and each entry in the TTree corresponds to an event recorded by the DDC. A program called “BinToRoot” processes each DDC binary file, loops over events, and records each channel waveform to a corresponding branch in an output ROOT file.

Once the ROOT files (**.root**) are created, we perform actual waveform analysis on the

data and produce a set of useful quantities. A code simply called “ProcessWaveforms” uses a custom “Events” class to load event waveforms, perform pulse finding and signal classification, and produce a set of “reduced quantities” (RQs) that are written to a new ROOT file format (.rq.root). These quantities may then be loaded by a waveform viewer (ShowWaveforms) and plotting script (PlotRQs) for visualization. Furthermore, these last two codes conveniently share a “RQs” class which loads the reduced quantities for events which pass a user-defined set of cuts.

7.3.2 Pulse Finding and Classification

The ProcessWaveforms code forms the base of our analysis, as it combs the waveforms for “pulses” (signals that rise above a noise threshold) and classifies these signals based on their shape. LG and HG channels are separately processed and their parameters are tuned independently to obtain the best results in their intended range of applicability. The LG channel has the largest dynamic range but is most useful for studying high energy signals, whereas the HG channel saturates even for moderate-energy signals but is sensitive to very small signals. The algorithm described in this section applies to both LG and HG.

The code uses global processing settings which specify PMT channel information, PMT gains as measured from PMT calibration, and pulse finding parameters. The code loads the input ROOT file, and for every event performs the following sequence:

1. Calculate the average baseline amplitude *for each channel* using the first and last μs of the waveform. If there is excessive deviation, the event is flagged for later exclusion.
2. Sum all four PMT waveforms to produce a temporary waveform, including baseline subtraction for each channel independently.
3. Sum the TPMT channels, then process the summed top PMT waveform with a special S2 filter, producing a filtered waveform (see Fig. 7.6).
4. A pulse finding function passes over the filter waveform. Windows where the waveform

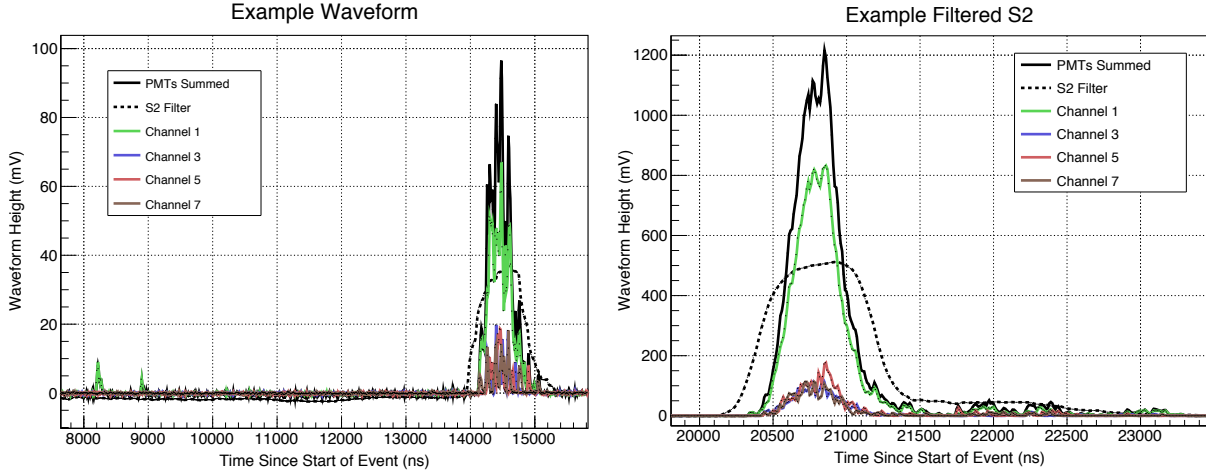


Figure 7.6: (Left) An example low-energy waveform in the LG channel, with each PMT trace, the summed waveform (black) and arbitrarily scaled S2 filter (dotted) shown. (Right) The S2 filter shown for a larger S2.

passes above a S2 threshold are defined as possible S2 regions. Spurious S2 windows, where the max filter value does not meet an extra threshold requirement, are removed.

5. Use the same pulse finder to comb the *total* summed waveform of all PMTs, finding signals that go above a fixed noise threshold. Merge any overlapping pulses.
6. Cluster and merge all pulses that overlap with the same S2 window, as well as those that are near the beginning/end of the S2 window.
7. Classify each summed pulse. Classify a pulse as S2 if it is overlapping with an S2 window. Else, if it has a continuous rise to its peak and doesn't "re-spike" above half-maximum during its fall, classify it as S1. Otherwise, classify the pulse as "Other".
8. Loop over all channels, and for each channel:
 - Process the individual PMT waveform with the pulse finder.
 - Merge any overlapping "peaks" (our term for a pulse found in a single channel).
 - Calculate per-channel, per-pulse RQs. For each peak found in a channel, find the summed PMT pulse it overlaps with, and apply the gain of that PMT channel to

calculate the contribution of that peak to the corresponding pulse area.

9. Calculate the remaining summed pulse quantities now that channel contributions are known, including the reconstructed xy position.
10. Record the RQs as vector-based structures to the output `.rq.root` file for each event.

A nice feature of the ROOT format is that we can store the output RQ data as dynamically-allocated vectors, i.e. we are not limited to fixed-length arrays. This is useful since we are dealing with events with arbitrary numbers of pulses. Note that we produce RQs at various levels: per event, per pulse, per channel etc. This means that our RQs are stored as scalars, vectors (dimension = # of pulses, # of channels), and 2D vectors (dimension = # peaks $\times$ # channels). Such a structure preserves useful low-level information.

Some words are in order about the philosophy of our pulse finding technique. The most relevant pulse quantities in our analysis, specifically the signal size (area) and classification, determine the order of operations. The S2 filter is used early in the algorithm because it determines how pulses in the event are clustered together, and the pulse structure fixes the dimensionality of the RQs. Furthermore, pulse-level quantities that are related to the pulse area must be calculated using per-channel PMT gains, so the peaks found in a given channel must be associated with a summed PMT pulse to tally its contribution. Pulse-level variables calculated directly from the summed waveform do not take into account the PMT gains, but are still useful for describing the timing or shape of the pulse.

The S2 filter, which comprises the majority of our pulse classification scheme, is done as follows. A moving window, or box, scans over all samples in the waveform and integrates all samples within that box. This box has a characteristic S2 width of $1\ \mu\text{s}$. A smaller box of characteristic S1 width (200 ns) scans over the S2 box and integrates the samples within this smaller window. The maximum S1 integration value within the S2 box is subtracted from the entire S2 window, so that only the wider S2-like component persists in the filtered waveform. The sliding S2 box integrates over a wide enough window that S2 tails are also captured, as shown in Fig. 7.6. The resultant S2 filter waveform, as well as the total summed

PMT waveform, may be optionally saved in the .rq.root files produced by ProcessWaveforms.

7.3.3 An Event Viewer for Hand-Scanning and Verification

In order to validate the performance of our pulse finder over hundreds of waveforms and inspect events of interest, it is necessary to have an event viewing tool. The ShowWaveforms code is an extremely useful event viewer which plots not only the individual PMT waveforms, but also pulse finder/classifier results.

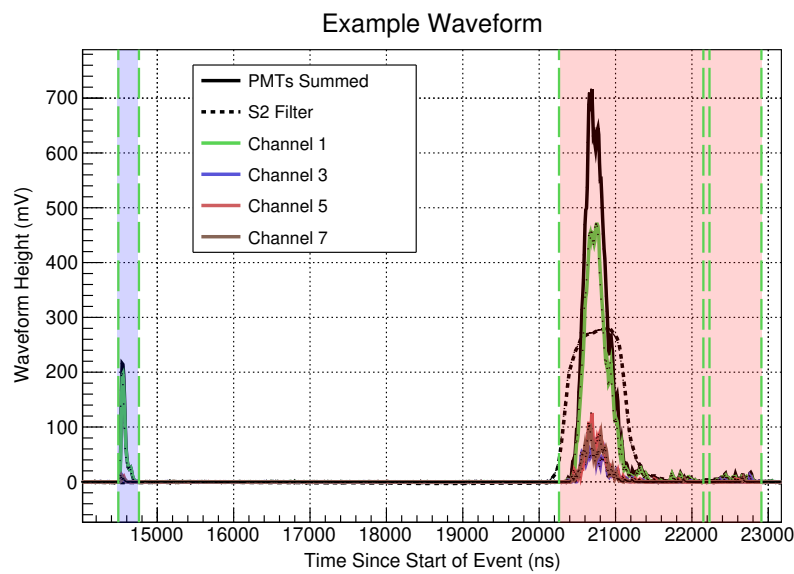


Figure 7.7: An example waveform displayed in the event viewer, with blue and red windows indicating S1 and S2 pulses respectively. The dashed green lines indicate the individual channel peaks contributing to the summed pulses.

The code runs as an interactive ROOT TApplication which requires at least a ROOT file containing the PMT waveforms. The program reads this input file, loads the waveforms, and plots them as overlaid graphs in the application window. Run time options allow for the user to plot a single specified event, loop over and display all events automatically at some fixed frequency, or move between events with keyboard input. Another option allows the user to select specific PMT channels for viewing.

If the user provides an RQ file containing the output of ProcessWaveforms, the application

will draw not only the individual PMT waveforms, but also pulse windows which are colored based on their classified pulse type (blue windows for S1, red for S2, and gray for “Other”). Dotted lines corresponding to the contributing peaks are also shown for a select channel. Furthermore, if the .rq.root files contain the summed waveform and S2 filter waveform, these will also be plotted in the application window (see Fig. 7.7).

All RQs are made accessible to this code via a “RQs” class, which is shared with the PlotRQs code. An important related feature is that the RQs class contains a set of parameters which allow for implementing cuts on the reduced quantities, such as S1 pulse width, S2 reconstructed position, number of pulses in an event, etc. For any cuts that are activated, both ShowWaveforms and PlotRQs will exclude any events not meeting the cut criterion, which allows looping over a desired subset of events. This avoids many hours of manual data selection and ensures consistency across the data visualization codes.

7.4 Calibrations of the DAX TPC

Prior to implementing a ^{206}Pb source in the DAX TPC, we performed dedicated calibration runs to characterize the detector response. This is crucial, since we want to quantify ^{206}Pb yields in a meaningful way that is relatable to other experiments and existing models.

For our main calibration run, we installed a source rod with deposited ^{109}Cd to produce low-energy ER events in the TPC. Prior to filling the detector with Xe, the PMTs are operated in vacuum to perform a PMT calibration as described in the next section. Following the PMT calibration, the detector is filled with LXe to the desired level and tuned to stable conditions (which would subsequently be used for ^{206}Pb runs). An external ^{57}Co was then used to estimate the purity of the Xe during our calibration run, and was removed in order to acquire data of the internal source alone at a variety of drift fields. We then perform a Doke analysis to obtain g_1 and g_2 parameters. Our data acquisition and processing procedures have already been described.

7.4.1 Gain Calibration of the PMTs

The digitized PMT waveforms recorded by the DDC-10 are ultimately back-converted into time units of ns and amplitude units of mV during waveform processing. Pulse integration therefore produces area units of mVns, which is converted into more physical units by understanding the PMT response to single photons.

A single photon produces a photoelectron in the PMT photocathode via the photoelectric effect, and this photoelectron is then drifted with an electric field through the internal vacuum space towards a stage of dynodes. After hitting the initial dynode, electron multiplication occurs so that multiple electrons hit the next dynode, and the process repeats for many dynodes. The number of electrons produced from the initial photoelectron results in a large output current; the amplification of the initial photoelectron is called the *gain*. A PMT base circuit provides high voltage to each dynode in order to produce the necessary internal fields, while also providing signal pickoff from the final stage.

However, photocathodes don't produce one photoelectron (phe) for every incident photon. Photocathodes have both a quantum efficiency and probability of double phe emission which are wavelength dependent and vary from PMT to PMT (see Sec. 6.3.1). We do not perform dedicated measurements of these quantities for our PMTs, so we will adopt values from literature when necessary, and characterize our PMTs with a simple gain calibration using dark counts (thermal photoelectron emission from the photocathode) at room temperature.

With our light-tight detector space at vacuum ($\approx 10^{-6}$ mbar), we bring all PMTs to operational voltage with the TPC grids unbiased. We then adjust the trigger settings of the DDC-10 such that for each PMT, the majority of triggers in the corresponding high gain channel result in noise and the remaining triggers show a dark count pulse. This is done to avoid biasing our measurement of the single phe response. For every trigger, both high gain (HG) and low gain (LG) channels are simultaneously recorded for all PMTs.

These waveforms are recorded as 10 μ s windows and the resulting data is then processed using ADAX. A modified ProcessWaveforms code combs over all recorded waveforms and integrates all pulses which rises over an absolute threshold, which is set just above baseline

noise. To avoid biasing, if no pulse is found above threshold, the largest amplitude value in the waveform is taken to be a pulse and integrated. This analysis is performed for each dataset of 10^6 triggered events, with the PMTs held at a different bias voltage for each dataset. A ROOT script is then used to histogram the integrated pulse areas for each PMT.

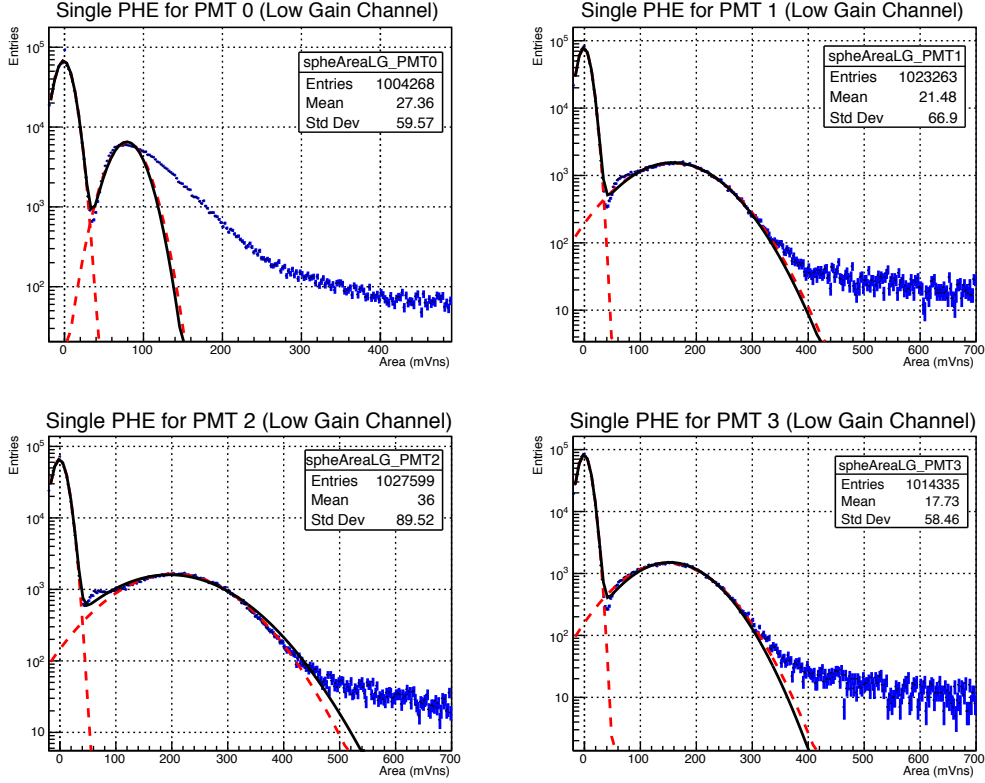


Figure 7.8: A measurement of the single photoelectron spectrum for four DAX PMTs biased at 900 V in the low gain channel. Shown are initial fits (red) and total summed fit (black).

For each PMT histogram, a series of fits is performed using ROOT analysis software. First, preliminary Gaussian fits are done independently on sub-ranges of the histogram for both the pedestal (noise) peak and the single phe (signal) peak. These preliminary fits yield parameters which are then fed into a sum of two Gaussians, which is re-fit to the overall distribution. The initial fits and final overall fit for each PMT in the LG channel are shown in Fig. 7.8, for a PMT bias voltage of 900 V.

The Gaussian fits perform quite well for the 1-inch TPMTs, however this model clearly does not capture the full response of the 2-inch BPMT (PMT0). A separate procedure is

therefore adopted for the BPMT, whereby a truncated Gaussian is fit to a sub-range of the distribution to capture the trailing edge.

For the special case of a Gaussian truncated from the left at the origin, the probability density function (PDF) is given by

$$\phi'(x) = \frac{1}{\sigma Z} \Theta(x) \phi(x), \quad \phi(x) = \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right]$$

where μ and σ are the mean and standard deviation of the normal Gaussian and Θ is the step function forcing the PDF to 0 for $x < 0$. $Z = 1 - \Phi(\alpha)$ is a variable of the Gaussian cumulative distribution function (CDF) Φ , where $\alpha \equiv (a - \mu)/\sigma = -\mu/\sigma$ for a Gaussian on the interval $[a, b) = [0, \infty)$. The CDF is given in terms of the Gauss error function:

$$\Phi(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x}{\sqrt{2}} \right) \right]$$

The mean of the truncated Gaussian is then calculated from

$$\mu' = \mu + \sigma \frac{\phi(\alpha)}{Z}$$

This model is found to work significantly better, as the measured gain values for both the top and bottom PMTs show approximately the expected ratio of 10 between the LG and HG amplifier channels. However, the bias voltages 750 and 800 V for the BPMT yielded unmeasurable gains in the LG channel, so these two points were extrapolated from the HG channel using this expected factor of 10 between amplifier channels. The resulting gain values for all bias voltages are shown in Fig. 7.9.

For all PMTs, there appears to be an upward systematic bias of the single phe response in the LG channel at low bias voltages. This is due to the single phe peak merging with the noise peak, throwing off the fits. Since the higher voltages provide more reliable gain measurements and optimal signal-to-noise ratio in our single phe response, we bias our TPMTs at 850 V and our BPMT at 900 V for the measurements shown in this chapter, giving near-equivalent PMT gains of $\approx 3 - 4 \times 10^6$ in the HG channel.

The absolute gain, or the amount of charge measured from a single phe, is calculated from the integrated pulse area using known values from the PMT circuit. The average single phe

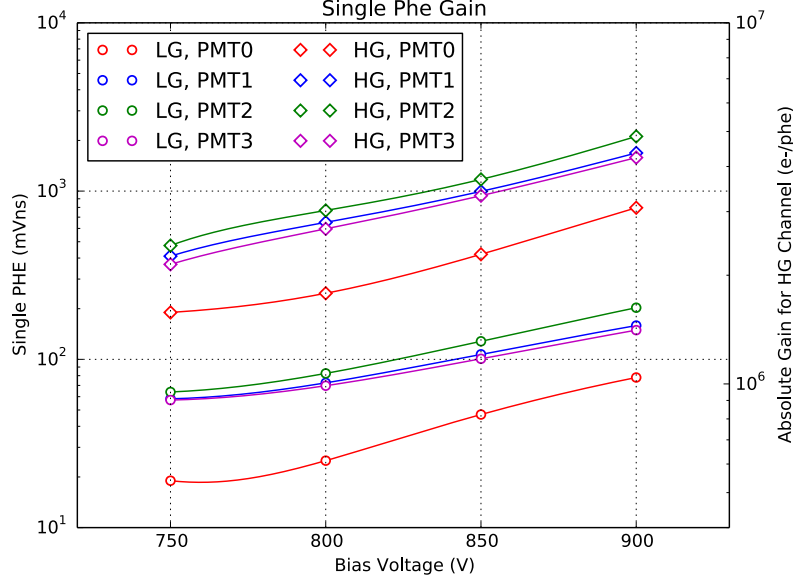


Figure 7.9: Gain dependence on bias voltage, for all PMTs in both low and high gain channels. The first two points for the BPMT (PMT0) are not measured, but extrapolated from the HG channel as described in the text.

pulse area $\langle A \rangle$ may be related to the current I passing through an input resistance $R = 50 \Omega$ at the amplifier:

$$\langle A \rangle = Vt = \frac{VQ}{I} = QR$$

Using the factor $C = 1.6 \times 10^{-19}$ to convert charge Q from Coulombs to total electrons, and accounting for the known amplifier gain on the measured signal, we obtain the PMT gain:

$$G_{\text{abs}} = \frac{\langle A \rangle}{RCG_{\text{amp}}}$$

7.4.2 Assessing Purity and Position Reconstruction with ^{57}Co

After acquiring PMT calibration data with the detector at vacuum, the thermosiphon cool-down is initiated and the detector is filled with LXe to the desired liquid level (we estimate a gas gap of $2.2 \text{ mm} \pm 300 \mu\text{m}$). The liquid level was used in order to optimize our extraction efficiency while limiting the gas gain (to ease PMT saturation issues). The remainder of the calibrations discussed in this section were performed after achieving stable detector conditions.

Constant recirculation is needed to maintain purity as the detector components outgas, and electronegative impurities such as O_2 are largely removed with the getter. We assess the purity (or electron lifetime τ) using a source which produces events throughout the drift region, since the number of electrons which reach the liquid surface has an exponential dependence on the drift time:

$$Q(t) = Q_0 e^{-t/\tau} \quad (7.4.1)$$

Our low-energy internal source (described in the Sec. 7.4.3) is highly localized to the fused silica rod, so it is not ideal for studying the full drift distribution. We use an external ^{57}Co disk source placed just outside the outer vacuum can at the approximate height of our active LXe volume. This provides γ lines at 122 and 136 keV, which are just high enough to penetrate into the active region and still undergo full photoabsorption.

Calibration data is simultaneously collected for both the internal and external sources. Several small-scale iterations of signal processing are performed on the data to tune the ADAX pulse finder and classifier through visual waveform inspection. By processing a large calibration dataset and examining the resulting pulse populations, we verify that ADAX performs sensibly on data *en masse*.

Fig. 7.10 shows area-width plots for the various classified pulse types in the low gain channel. Most importantly, our pulse-finding and classification codes are good at separating S2 pulses from S1s with tails and “other”-type pulses (low, spiky pulses which are small clusters of electrons). These plots do not just include the primary S1 and S2 “trigger” pulses, but all pulses found within all events. They therefore provide the full range of S1 and S2 signals detectable by our pulse-finding algorithms; it appears that have a near-single phe S1 threshold and a sub-50 phe S2 threshold.

Unfortunately, ^{57}Co events lie near the boundary for PMT saturation at 122 keV, since the light produced is concentrated in just four PMTs. Particularly for large S2 signals, the 2 V limit of the DDC unit is insufficient and the signal is clipped. To minimize S2 saturation, ^{57}Co data is acquired at low fields (100 V/cm). Since the BPMT window has a much larger active area than any single TPMT, its saturation is unavoidable; however, we are still able to

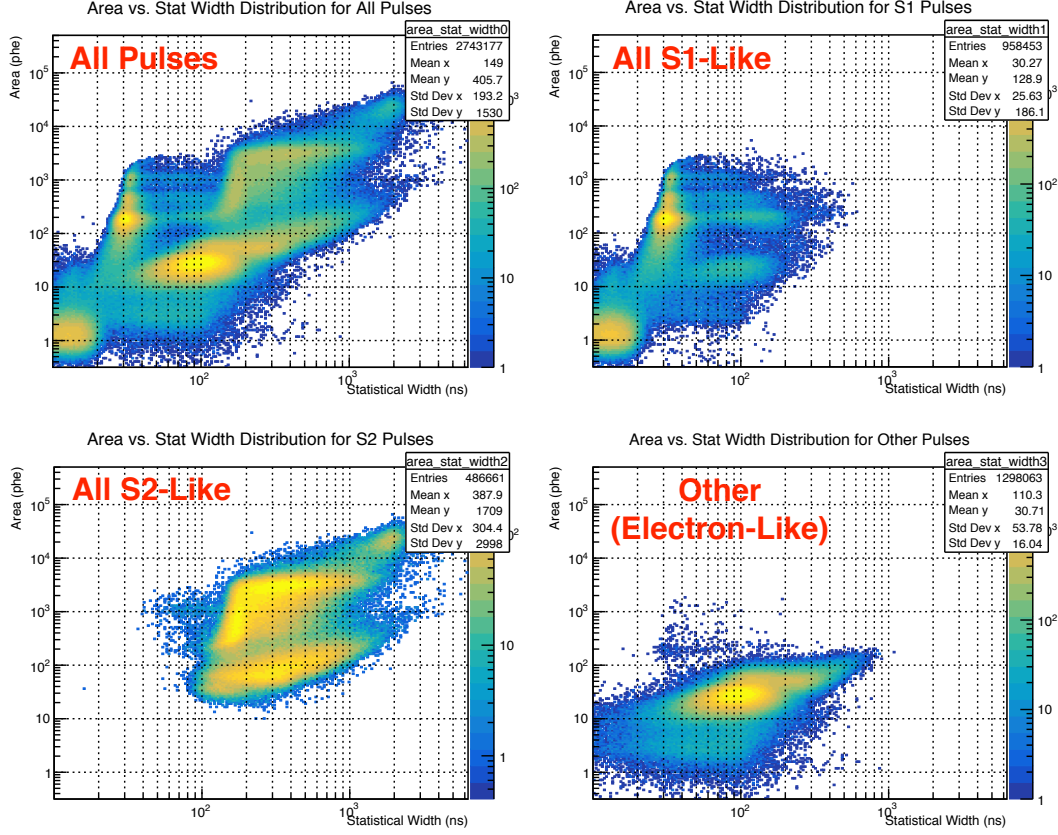


Figure 7.10: Pulse area–width distributions for all events found in a $^{57}\text{Co} + ^{109}\text{Cd}$ dataset. (TL) all pulses, (TR) all S1-like pulses, (BL) all S2-like pulses, (BR) all “other”-type pulses.

obtain useful signal information using the TPMTs alone, including validation of our position reconstruction algorithms and purity measurements.

Fig. 7.11 shows the reconstructed centroid and corrected centroid xy positions of calibration events, after applying a cut which removes events with a saturated BPMT. We obtain a clear visualization of both our localized low-energy internal source and our external source, with a position distribution that is very similar to that expected from BACCARAT simulations (Sec. 6.3.2). The external source produces a 122 keV γ , which has a short penetration depth in LXe ($\lesssim 1$ cm [129]). These events are therefore concentrated in the periphery of the detector, explaining the clear separation shown in Fig. 7.11. Furthermore, the positions of the ^{57}Co events match expectation based on the known physical locations of the TPMTs.

By isolating ^{57}Co events across the drift range, we can also calculate the purity of our

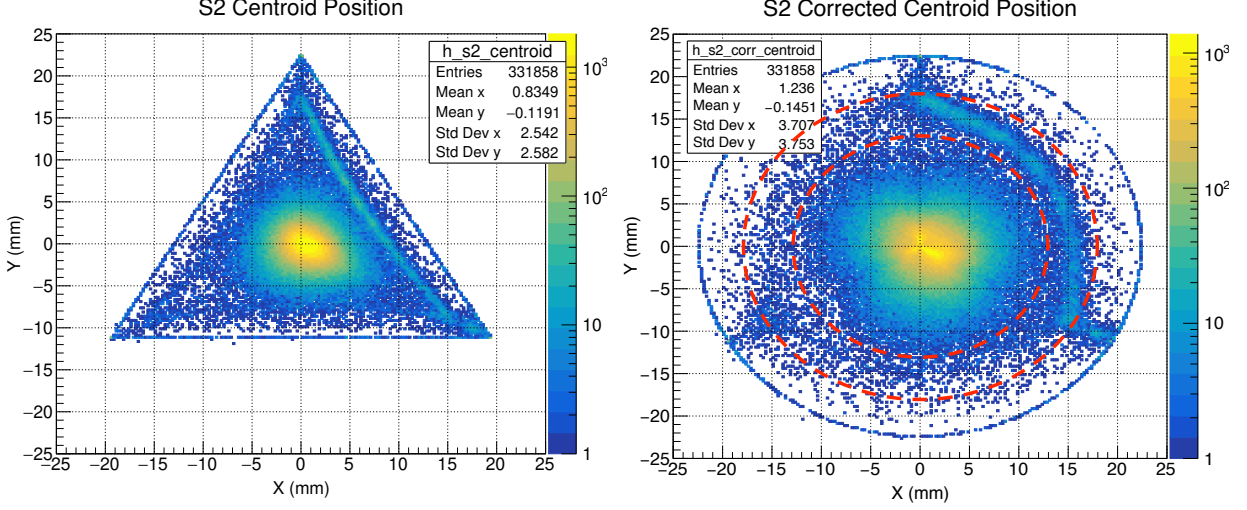


Figure 7.11: Reconstructed positions of ^{57}Co external source events and ^{109}Cd internal events. Red dashed lines indicate selection cut for ^{57}Co events in corrected position space.

LXe. To do this, we implement an additional cut on the peripheral events, as shown in Fig. 7.11. Events with a corrected centroid radius $13 < r < 18$ mm are selected, and their drift dependence of the S2 size (in TPMTs only) is shown in Fig. 7.12.

Exponential fits to these distributions is performed over various sub-ranges, giving a small variation in the electron lifetime. For our ER calibrations, we adopt the value $\tau = 28 \mu\text{s}$, since this corresponds to the most local drift time measurement at the location of the rod ($6 \mu\text{s}$ at 100 V/cm) and minimizes the interference of systematics due to field variation in the periphery.

This purity is rather poor compared to other LXe experiments, which typically achieve $\tau > 100 \mu\text{s}$. This can be explained by the very low recirculation rates used in the calibration run; the recirculation rate through the MFC was lowered to 0.8 slpm to minimize potential liquid level oscillations, after an initial purification at 1.5 slpm for many days prior to data taking. This issue was later resolved, so that higher purification rates could be used during our ^{206}Pb run.

Given the very small drift length of our TPC ($\approx 6 \mu\text{s}$ between the source rod and the gate), we still achieved reasonable S2 yields in the calibration run. Though the resolution

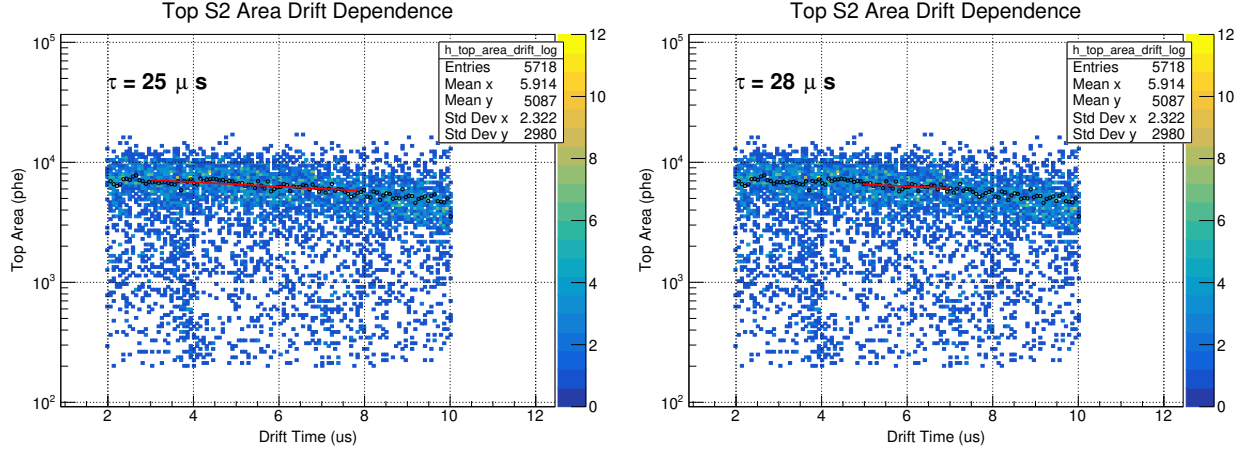


Figure 7.12: Electron lifetime fits to various sub-ranges of the S2 drift dependence: (left) from $3 - 8 \mu\text{s}$, (right) from $5 - 7 \mu\text{s}$. The fit on the right is used for the ER calibration.

is diminished, we can use the exponential fit from calibration data to perform an electron lifetime correction to correct our detector parameter g_2 .

From the COMSOL simulation shown in Fig. 6.15, we saw that the drift field within 5 mm of the TPC wall may deviate by $\pm 20\%$ from the mean drift field depending on the depth. NEST models give that such large overall fluctuations in the field can result in $\sim 5 - 10\%$ deviations in the observed S2 signal. Higher fields at low drift times, and vice versa, may skew the drift dependence of the S2 size and worsen the purity estimate. There is some uncertainty in our purity, however this is minimized by fitting the ^{57}Co distribution over a shortened drift range local to the rod.

7.4.3 Localized ER Calibrations with a ^{109}Cd Source

To calibrate the detector, it is important to use a well-understood, well-constrained radioactive source so that we may solve for unknowns in our detector response. Sources of electron recoil (ER) events, such as γ or β sources, are commonly used in Xe detectors to understand detector response across a very wide span of energies and in a variety of ways. These sources may be implemented as isotropic disk sources, collimated beams, or injected sources which are uniformly distributed (as discussed in Section 3.3.1).

We designed a TPC to characterize a ^{206}Pb source, with a low-yield signature suspected to be comparable to potential WIMP signals at low nuclear recoil energies; we therefore want to calibrate our detector with a low-energy ER source. Furthermore, since ^{206}Pb events are expected to be highly localized to the surface of the source rod, low energy X-rays provide a somewhat comparable measure of our important detector parameters g_1 and g_2 (which in general vary across the detector).

To achieve this, we implemented a ^{109}Cd source rod using the exact same techniques as for our ^{206}Pb source. This rod was used in our calibration run, in which our detector parameters were set as precisely as possible and maintained through the subsequent ^{206}Pb runs. ^{109}Cd undergoes electron capture and produces just a few lines in the desired energy range: a 88 keV γ for studying moderate-energy photo-absorption, a prominent 22 keV X-ray line for calibrating the detector at a low energy, and a 3 keV X-ray for testing the low-energy limits of our signal chain. While we find the 3 keV line to be discernible in the high gain channel, we will focus on the calibration of our low gain channel using the coherent 22 keV population; we ultimately use the low gain channel to perform our ^{206}Pb measurements.

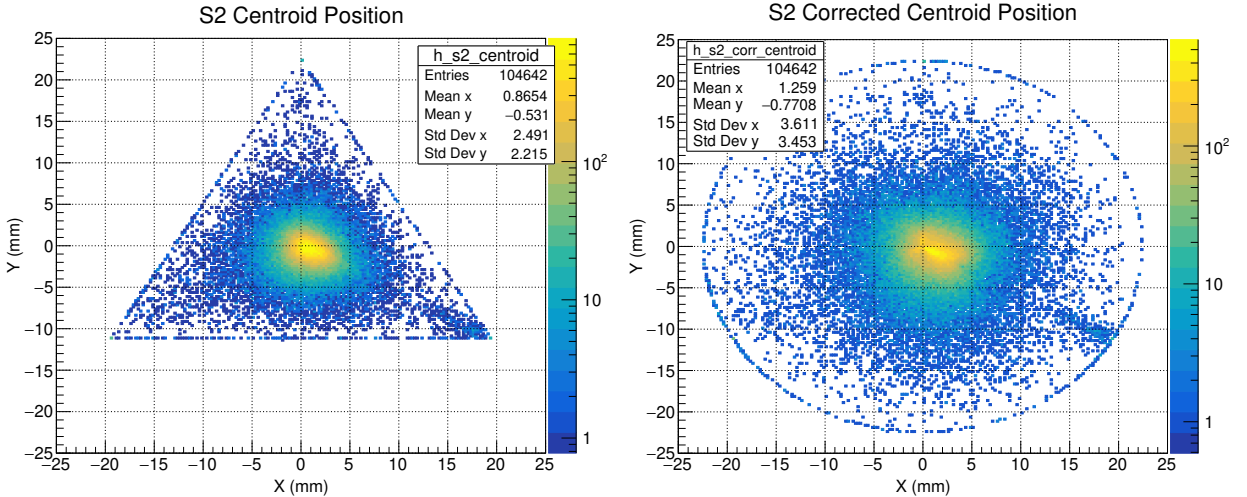


Figure 7.13: Centroid and corrected centroid xy position reconstruction of ^{109}Cd events.

The simplest set of cuts we make on the calibration data, which we will refer to as our “minimal cuts”, involves cutting on the number of S1 and S2 contained in an event. To

isolate “clean” events in general, we require only 1 S1 (with at least 2 PMT hits) preceding an S2, and 1 or 2 S2 (to allow for the possibility of photoionization of the cathode, which we found to be likely based on drift localization of secondary S2s).

Fig. 7.13 shows the xy localization of our source using our position reconstruction algorithms. These algorithms use the top PMT hits to calculate both centroid and corrected centroid xy as described in Sec. 6.3.2. As we can see, both algorithms work as expected based on BACCARAT simulations. It is quite encouraging that our source is both centralized and shows the most spread along the physical axis of the rod, as we would expect. Furthermore, the orientation of the rod is correct based on the known position of the PMTs (notice that the rod entrance hole is located beneath the bottom-right PMT).

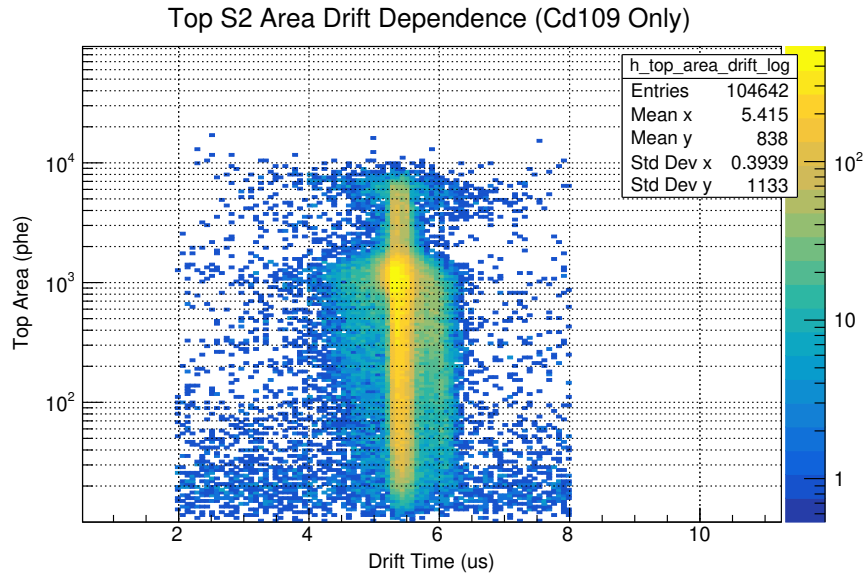


Figure 7.14: Drift time distribution of S2 from the ^{109}Cd source.

We may assess the drift localization of the source by looking at the drift time between the primary S1 and S2. Figure 7.14 shows the drift distribution as a function of the “top area” (the sum of pulse areas in the TPMTs). The TPMT area is used here and in general for higher energy signals, since the 88 keV γ events from ^{109}Cd easily saturated the bottom PMT signal.

Taking the S2 size as a rough proxy for energy, we can see that higher energy signals

have more spread in the drift time distribution due to the γ having a higher penetration depth in LXe. In general, however, the drift time distribution shows clear localization to the z position of the source rod. The events are highly concentrated within $< 0.5 \mu\text{s}$ at a drift time of $\approx 5.4 \mu\text{s}$, which matches the expected depth of our source rod at a drift field of 500 V/cm. This allows us to reliably create a tight drift time cut to localize and select a pure sample of source events.

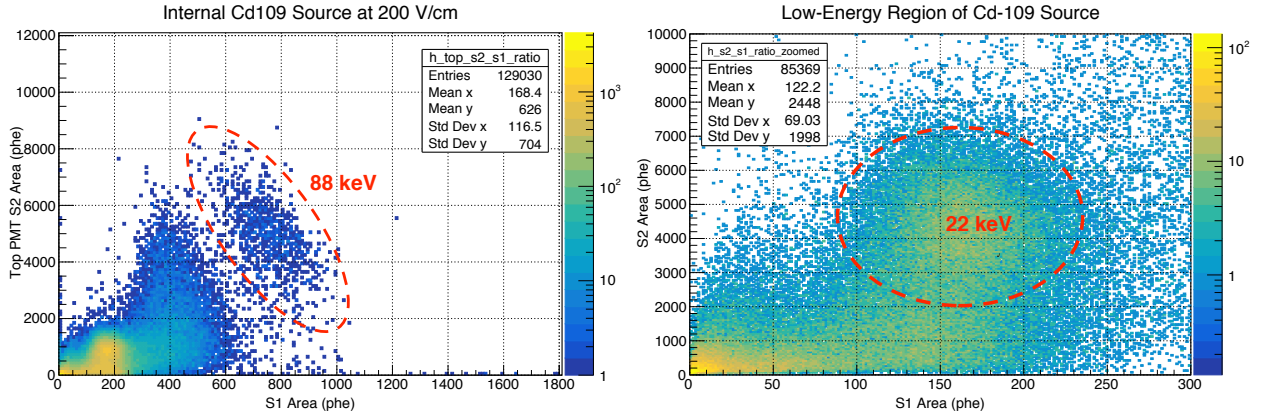


Figure 7.15: The various populations from ^{109}Cd are shown in (S1, S2) space.

After selecting “rod events” with a drift cut ($\pm 0.5 \mu\text{s}$ about the mean), we investigate the energy spectrum by looking at (S1, S2) space. As discussed in Sec. 4.1.2, we expect to see an anti-correlation between S2 and S1 due to recombination physics. We see this in the highest-energy population in Fig. 7.15 (left), which is presumably the 88 keV γ photo-absorption line. Our ability to resolve this anti-correlation indicates a reasonable energy resolution (i.e. fluctuations in our light and charge collection do not dominate our resolution).

Given the known relative branching ratios for the 3 keV X-ray ($\approx 10\%$), 22 keV X-ray ($\approx 85\%$), and 88 keV γ ($\approx 4\%$) from Cd, we can assign energies to the 3 main populations and cross-check with NEST. The population with the highest frequency corresponds to the 22 keV X-ray, which is just barely separable from the messy low-energy X-ray spectrum. Running NEST simulations over a range of reasonable g_1 and g_2 parameters verifies that the observed yields are reasonable at the measured purity. By measuring the mean S1 and S2 yields at a known energy, we can perform a detector calibration.

Specifically, we use the Doke method to leverage recombination physics to determine our detector response parameters g_1 and g_2 . This is done by acquiring ^{109}Cd datasets over a wide span of drift fields and performing the following procedure at each drift field:

1. Perform a drift time cut based on the appropriate drift range for each drift field.
2. Do a 10 mm-radius fiducial cut in xy to effectively remove peripheral backgrounds.
3. Select the central population of 22 keV events in (S1, S2) space (see Fig. 7.15).
4. Project these events onto the S1 and S2 axes and fit a Gaussian to each distribution to obtain S1, S2 means. Also extract the σ and parameter error from each fit.
5. Plot the mean yields from all drift fields in (S1, S2) space and fit with a line to extract g_1, g_2 as discussed in Sec. 4.1.2.

The results of this procedure are shown in Fig. 7.16.

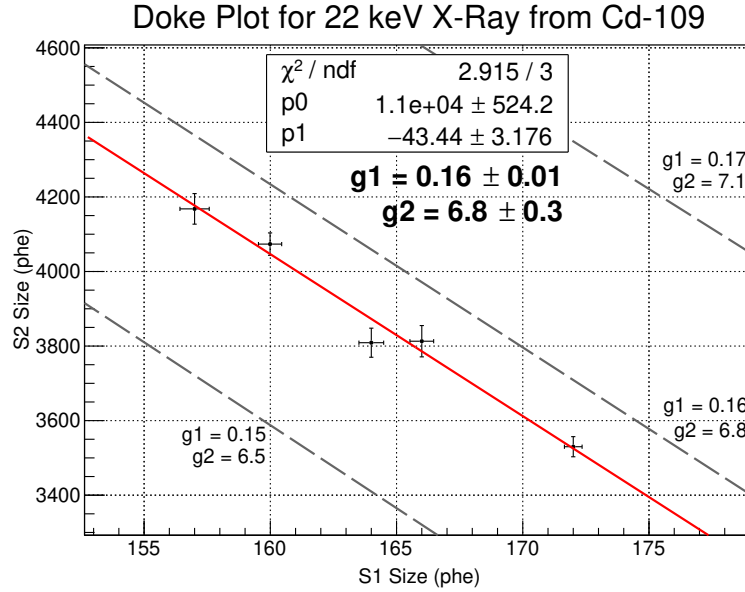


Figure 7.16: The mean S1 and S2 yields for drift fields $\approx 200 - 500$ V/cm with error bars, a linear fit (red), and measured g_1 and g_2 with errors. NEST v2 prediction lines are shown (dashed) for g_1, g_2 parameters spanning the full error range.

The measured $g_1 = 0.16$ phe/photon is low compared to the $g_1 = 0.19$ obtained from LCE simulations once we account for double photoelectron emission (see Sec. 6.3.1). This is reasonable given the idealized simulation detector model, which doesn't include all of the “holes” in our detector geometry and overestimates the active region of each PMT window.

The g_2 parameter is more difficult to validate, since it depends on a number of other independent detector parameters: extraction field, gas gap, gas pressure, and geometric light collection efficiency in the gas region (g_1^{gas}). These dependencies were discussed in Sec. 6.4.3, and are built into the NEST simulation software. Therefore, we may use NEST to cross-check our yields for a constrained range of detector parameters.

However, our g_2 is measured with the assumption that all electrons make it to the liquid surface from the interaction site (i.e. $\tau \rightarrow \infty$). From our electron lifetime measurements using ^{57}Co , we know this is not the case. If we correct our observed S2 signal to account for purity, our linear fit parameters change as follows:

$$\begin{aligned} \langle S2 \rangle_{\text{obs}} &= \langle S2 \rangle_c e^{-t/\tau} = \frac{g_2 E}{W} - \frac{g_2}{g_1} \langle S1 \rangle \\ g_{1,c} &= -\frac{bW}{mE} = g_1, \quad g_{2,c} = \frac{bW}{E e^{-t/\tau}} = \frac{g_2}{e^{-t/\tau}} \end{aligned}$$

Therefore, the purity correction does not affect g_1 , but does cause us to underestimate the light collected per *extracted* electron. Using the mean drift time of the source rod, our correction yields $g_{2,c} \approx 8.3$ phe/(electron produced).

By correcting g_2 , we can now factorize it into the extraction region parameters which are input to our NEST detector model:

$$g_{2,c} = \eta \psi \sim f_{\text{NEST}}(E_g, h_g, p, g_1^{\text{gas}})$$

Since we know (relatively precisely) our gas gap $h = 2.2$ mm, extraction field $E_g = 8.6$ kV/cm, and absolute pressure $p = 1.6$ bar, we tune the unknown light collection g_1^{gas} such that NEST calculates a g_2 which matches our measured $g_{2,c}$.

We then produce NEST simulations for 22 keV X-rays across a span of drift fields, and for a variety of g_1 and g_2 parameters spanning our uncertainty range. The S2 yields predicted

by NEST are reduced by the electron lifetime correction to give the expected *observed* S2 signals. The resulting NEST lines are shown in Fig. 7.16. Given the uncertainties in the true liquid level, extraction field, and purity, the NEST-predicted yields agree quite well; NEST curves are within $\approx 5\%$ of observations and well within g_1 , g_2 uncertainties, validating our measured detector parameters.

7.5 Characterizing the Yields of ^{206}Pb Nuclei

Once a successful ER calibration was performed for our source rod configuration, the detector was opened up and the source rod was swapped with a ^{206}Pb source rod, identically created.

No other changes to the detector configuration were made, and a new run was initiated with stable detector conditions as similar as possible to the calibration run. The main difference is that our purity was vastly improved in the ^{206}Pb run, as a much higher recirculation rate (1.5 slpm, near the limit of our system) was maintained throughout the run. This ensures a much smaller correction to the S2 size.

Unfortunately, after recirculating for many days and beginning the data acquisition process, it was discovered that one of the top PMTs (TPMT 2) was faulty. It produced negligible output, essentially unchanged as the PMT bias was varied. This indicates either a bad internal connection or a completely compromised PMT, either way not externally fixable.

This eliminated the possibility for radial fiducialization during our ^{206}Pb run and reduced our light collection in the top array. However, it was still possible to salvage the final ^{206}Pb run through drift localization and signal cuts to exclude obvious backgrounds. Furthermore, our previous calibration data provided a centered source with uniform PMT response, allowing us to extract the relative contribution of each top PMT and derive a signal correction factor so that we may still use our calibrated g_1 , g_2 parameters. Using the relative S1 and S2 contributions from just the top PMTs, we deduce that losing one top PMT results in a $\approx 5\%$ correction factor to signals originating from the xy center. This estimate will be used for the remainder of the ^{206}Pb analysis.

7.5.1 Tagging Associated α Signals from ^{210}Po Decays

All ^{206}Pb events in our detector are accompanied by a 5.3 MeV α particle. It is important for our analysis that we are able to tag α events and separate α -contaminated events from pure ^{206}Pb nuclear recoils. Full deposition α events, which are well-modeled by NEST, are expected to produce enormous yields at 5.3 MeV which easily saturate our PMTs.

A first-pass method for removing large α signals is to check for saturation of the PMTs (i.e. clipping at the max amplitude of the DDC, ≈ 2 V). However, based on the kinematics of the source rod, we expect a wide spectrum of energy depositions.

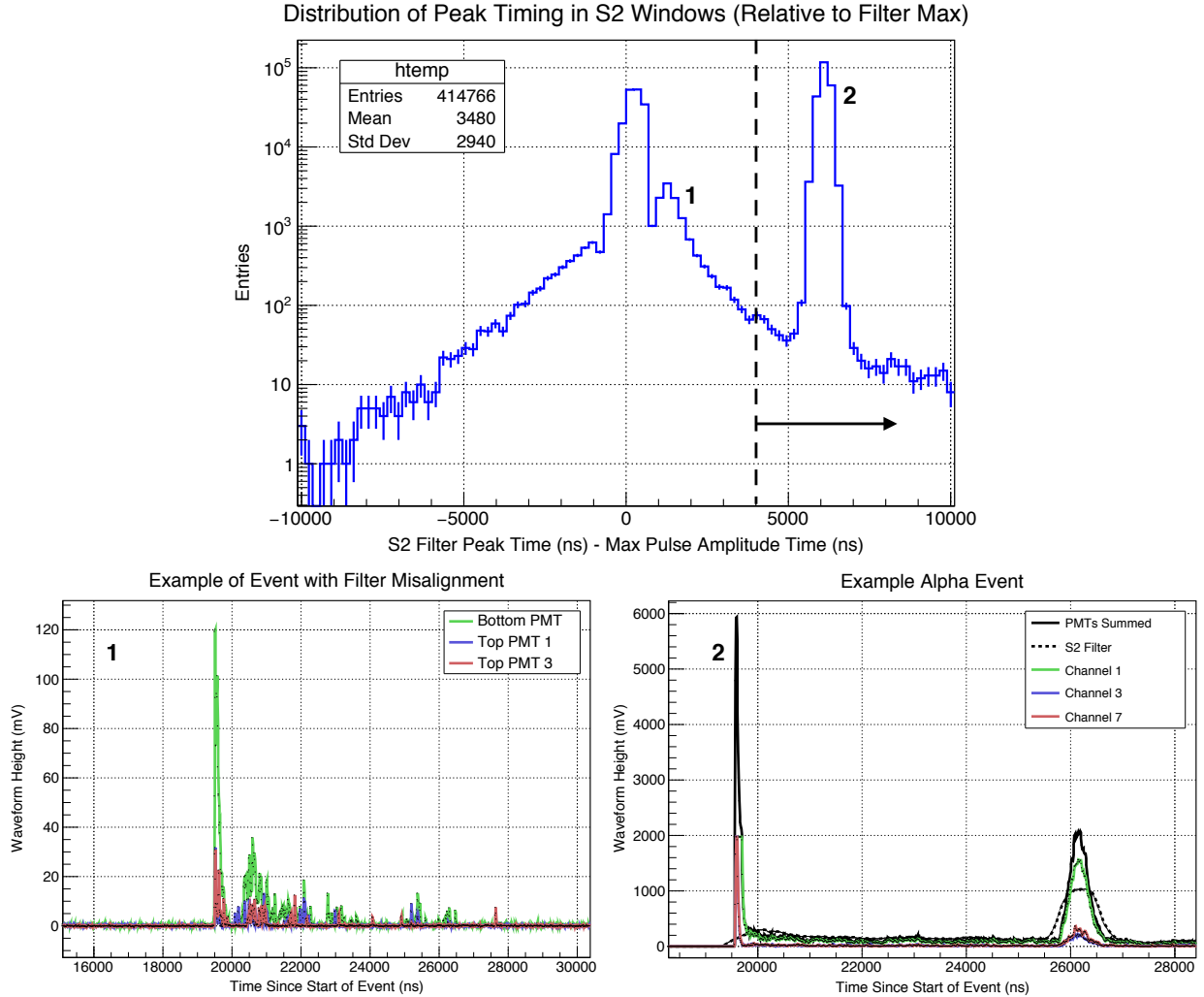


Figure 7.17: (Top) Time separation between the peak amplitude and peak filter value for all S2s, with α region indicated. (BL and BR) Example S2 pulses in populations 1 and 2.

Examination of sample α events revealed that our pulse finder was incapable of separating S1 pulses from S2 pulses, due to a large characteristic S1 tail that merged the pulses into a single classified S2 (see Fig. 7.17, bottom right). The S1 component saturates all PMTs and usually gives the highest waveform amplitude. The maximum value of the S2 filter, however, is reached within the window of the *actual* S2 component. Since the drift time between the S1 and S2 components of an α is fixed to the location of the rod, the difference in time between the S2 and S1 peaks gives a measure for tagging α events.

The distribution of this quantity, which we will call the “filter misalignment”, is shown in Fig. 7.17 for a ^{206}Pb dataset. We can classify events with filter misalignment $> 4\mu\text{s}$ as α events, and remove such events when isolating our ^{206}Pb candidates. It should be noted that while a saturation cut removes many such α events, this filter timing method is amplitude-independent and leverages the topology of the α waveforms.

In Fig. 7.17, we show example waveforms for two “misaligned” S2 populations. We see that in addition to the α waveforms (“Population 2”), there are also S2 pulses which have a smaller degree of filter misalignment (“Population 1”). These are mostly S1s with spiky S2-like tails, which is a poorly understood phenomena that is beyond the scope of this thesis; it may be either backgrounds at the liquid surface or secondary induced scintillation.

7.5.2 Selecting ^{206}Pb Events

Once α -removal cuts are applied to events containing α -like S2 pulses, we formulate additional cuts to select a clean sample of ^{206}Pb events. From Fig. 7.18, we see that there are 3 main coherent S2 populations in drift time.

Events from Population 1 are localized to the source rod, Population 2 is a surface population similar to that discussed in Sec. 7.5.1 (but with well-separated S1), and Population 3 events have enormous S2 and span most of the drift region. Fig. 7.18 shows examples for all of these populations, and examples of Population 3 at different drift times.

Population 3 is not localized to the source rod and has S2 signals which far exceed the charge yields predicted by NEST. We would expect ~ 20 electrons produced for a ^{206}Pb

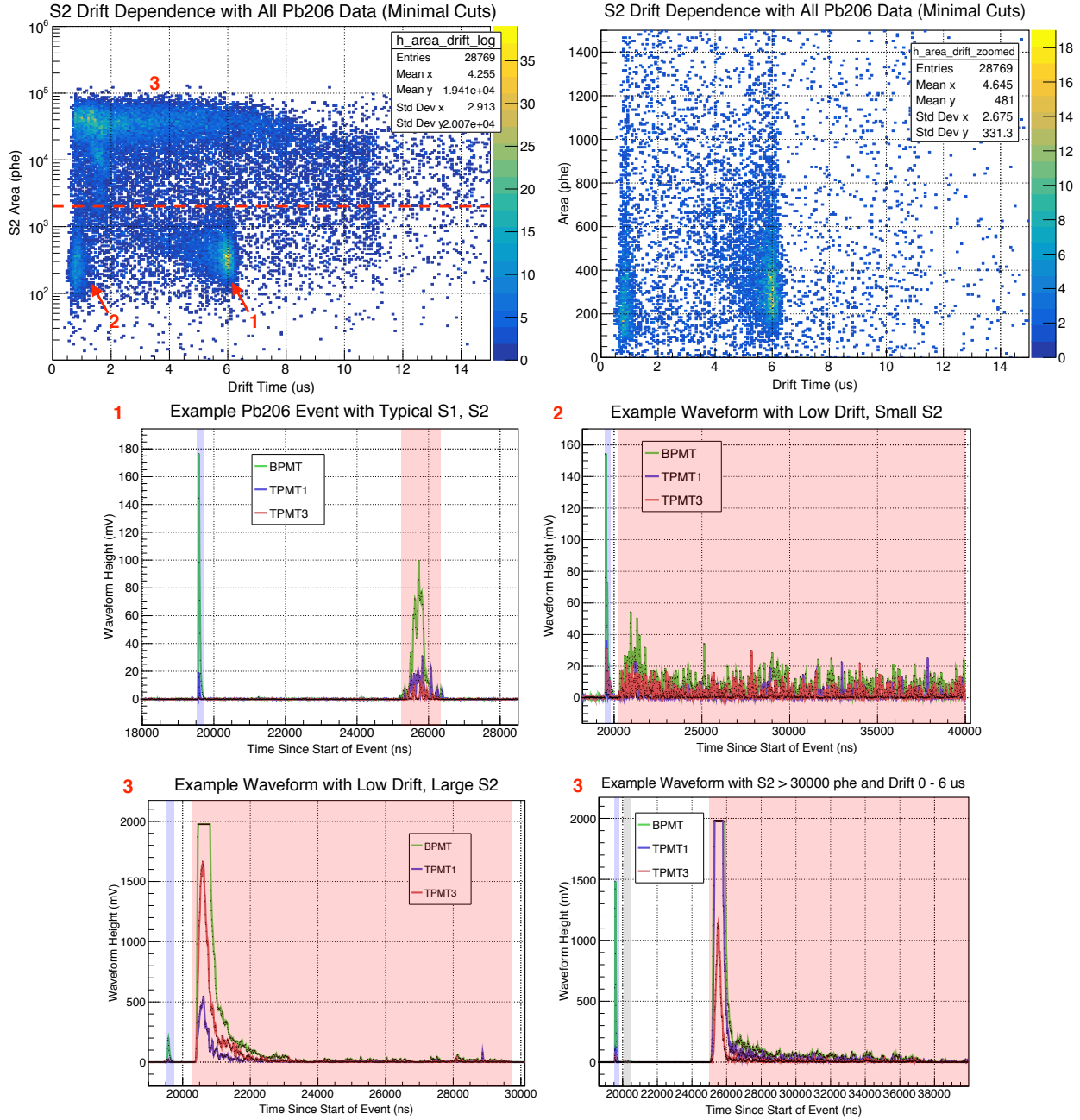


Figure 7.18: (Top) Drift time distributions (log and linear scale) for S2 populations in ^{206}Pb data. (Bottom) Example waveforms for all 3 drift time populations.

nuclear recoil, but using our measured g_2 (corrected) this population would yield $> S2/g_2 = 2000$ electrons. This population is likely due to external backgrounds as well as surface backgrounds from detector components, which would be more prominent in the gas phase and

near the liquid surface (at low drift times). It should also be noted that these backgrounds often show quite an asymmetric response between the remaining 2 top PMTs, which also indicates that they are non-fiducial/peripheral.

Population 2 is similar to the previous “Population 1” shown in Fig. 7.17, but with S2-like tails on the S1 that are actually separated enough to be classified as a separate pulse.

Population 1 from Fig. 7.18 shows a clean ^{206}Pb candidate event. To select all such events, we implement both a high-energy background cut ($S2 < 2000$ phe, or ≈ 240 electrons equivalently) and a drift time cut for depth fiducialization. The drift time cut is decided separately for each drift field dataset, using the mean of the drift time distribution after applying S2 cuts; events within $0.5\ \mu\text{s}$ of the mean are selected. The dependence of the mean drift time on electric field is shown in Fig. 7.19.

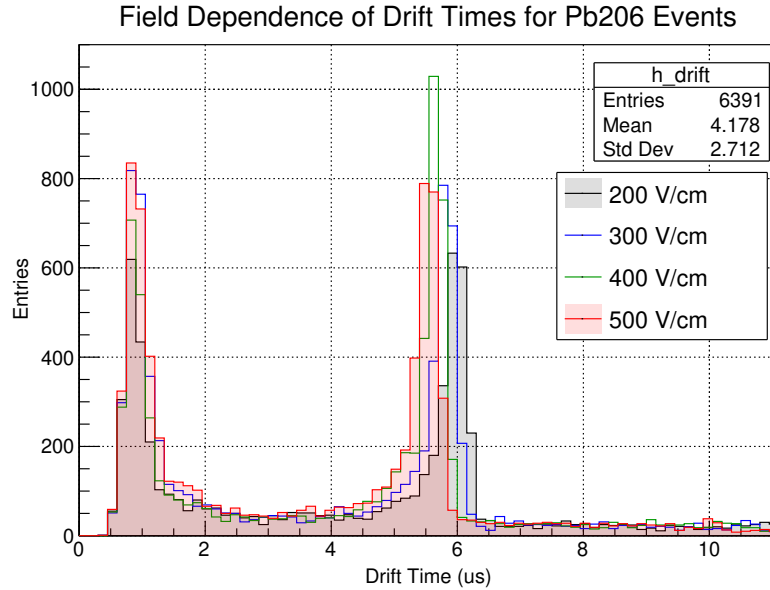


Figure 7.19: The drift time dependence of ^{206}Pb events as a function of the drift field.

The dependence of the drift time on electric field appears to agree with values in the literature [54]. However, these drift fields are not known with great precision, since COMSOL simulations were performed with an idealized detector geometry and leakage fields near the extraction region vary depending on the applied voltages. Our best assessment of field uncertainty from COMSOL simulations (even near the surface of the source rod, see Sec.

6.4.2) is $\approx \pm 25\%$, which is significant for the high-field data.

7.5.3 Comparing Yields with Existing Models and Data

We will now discuss our observed yields for ^{206}Pb nuclear recoils, and compare these results with NEST v2 simulations and previous WIMP search data from LUX.

^{206}Pb events are selected by implementing pulse saturation, α -removal, S2 maximum size, and drift time cuts as described above. A single S2 population remains after these cuts (shown at a drift time of $\approx 6\ \mu\text{s}$ in Fig. 7.18), however there are two remaining populations of S1 signals. The first population is a band at low S1 area up to ≈ 1000 photons; the second is a flat continuum up to our S1 cutoff, which will be discussed later. The corresponding S2 yield is ≈ 32 electrons.

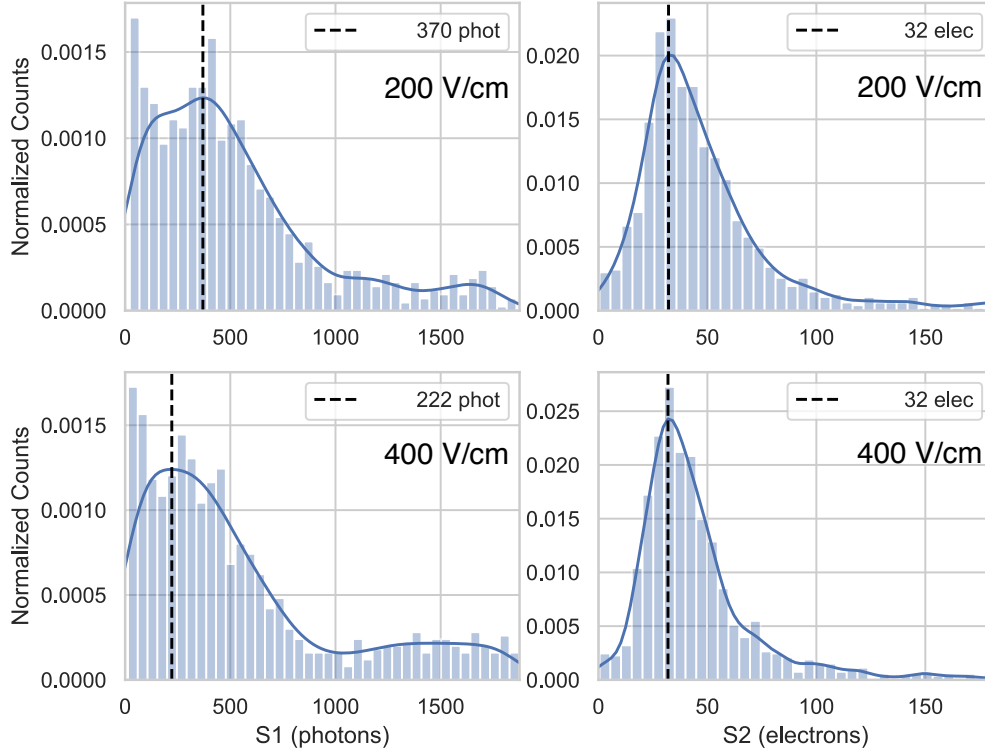


Figure 7.20: Light and charge yields (from measured g_1 and g_2) of ^{206}Pb at different fields. The maximum of the KDE curve serves as a proxy for the central value (black dashed).

Fig. 7.20 shows the light and charge yields for data at two approximate drift fields.

Histograms of ^{206}Pb events with Gaussian kernel density estimation (KDE) curves are shown, as well as the point of maximum KDE as a measure of central tendency. Since there is less uncertainty at lower fields and it will be easier to make direct comparisons with LUX data, we will primarily discuss the low-field (200 V/cm) data going forward.

Interestingly, the mean S2 signal has no discernible dependence on the global electric field. There is a noticeable change to the mean S1 yield at higher fields, which indicates that the local electric field magnitude at the interaction site is in fact changing enough to affect recombination. It is possible that there is S2 suppression due to post-recombination charge loss, however these results suggest that such charge loss mechanisms have more to do with intrinsic surface effects than with the relative location of the source within the detector. By design, our source is placed in the center of the detector, facing the PMTs, with field non-uniformities minimized. It is still possible, however, that local electric field variation and potential shielding effects at the source surface affect the drift of charge; ^{206}Pb travels < 100 nm in LXe (see Sec. 6.2), so electrons which survive recombination are similar distances from the deposited source layer.

As previously mentioned, two event populations persist after purity cuts. After applying an even tighter cut to remove the sparse tail of the S2 distribution (requiring $S2 < 100$ electrons), we plot the remaining ^{206}Pb events in discrimination space ($S1, \log_{10}(S2/S1)$). The resulting KDE plot in Fig. 7.21 shows two clear populations, with the right population being a continuum up to very large S1. It is unlikely that this larger population is a true ^{206}Pb component (e.g. a different charge state), since both S1 components have the same S2 yield. Furthermore, it was also discovered that this large S1 population runs all the way up to (and presumably beyond) saturation. This suggests that these are α -contaminated events in which the α nucleus penetrates partially into the LXe and contributes S1 light, but no S2. This would induce a broad, flat spectrum on the tail of the S1 distribution.

Since WIMP search regions are typically in a smaller S1 range, the inset figure in 7.21 contains a band with S1 from 0 – 200 phe. Mean discriminant values are calculated for various S1 slices of the band, and these means are fit with a power law function (the FOFOI

function of Woods [239]):

$$f(S1) = \frac{a}{S1 + b} + cS1 + d$$

The best fit is shown ($a = 18.1$, $b = 14.4$, $c = -0.0028$, $d = 0.648$), as well as 95% confidence intervals for the mean.

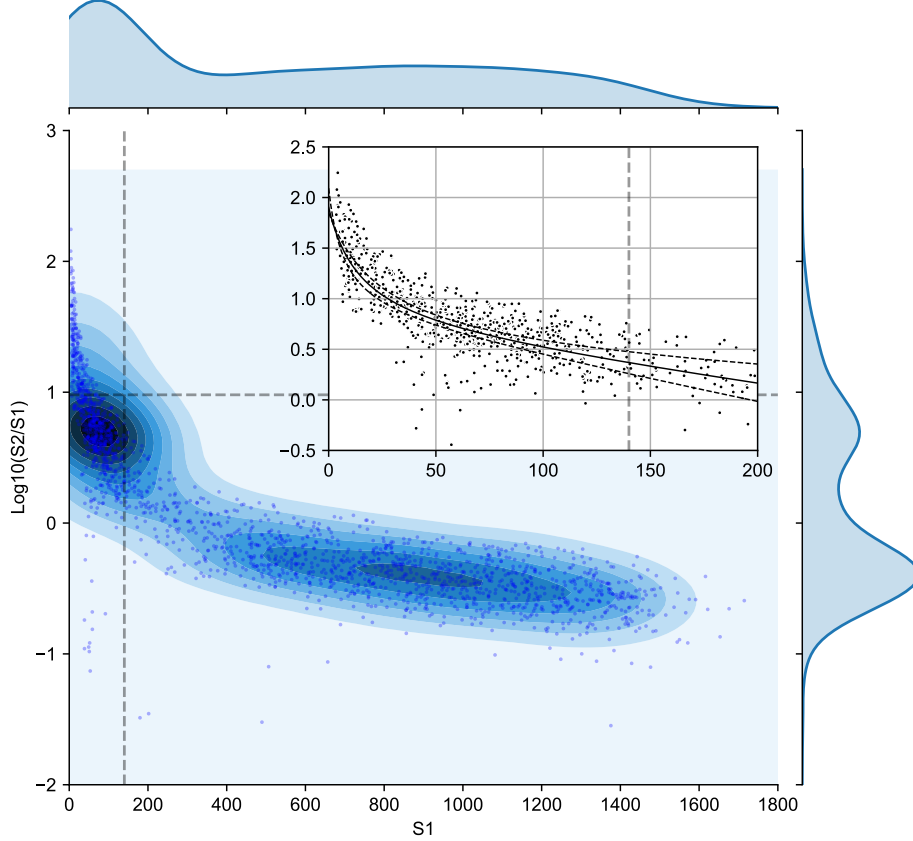


Figure 7.21: Scatter plot of ^{206}Pb events with KDE contours. Dashed grey lines give NEST v2 predictions based on the mean yields. A zoomed ^{206}Pb band with fit mean and 95% confidence intervals is inset, also showing the NEST prediction for S1 mean.

NEST v2 mean predictions for a full-deposition 103 keV ^{206}Pb nucleus (shown as grey lines in Fig. 7.21) give near-perfect separation of these S1 populations, and in fact appears to mark the endpoint of the observed ^{206}Pb band.

It is also important to investigate the discriminant quantity, since it encodes the interaction physics and is ultimately used to separate prominent backgrounds from WIMP-like NR events. In Fig. 7.22 we show the $\log_{10}(S2/S1)$ distribution for all ^{206}Pb events, and

mark the NEST v2 model predictions. Our hypothesis that the first peak corresponds to α -contaminated events is justified by the fact that the discriminant for this population is highly suppressed by the exceedingly large S1 component, so that it disagrees with the NEST predictions even for the α model.

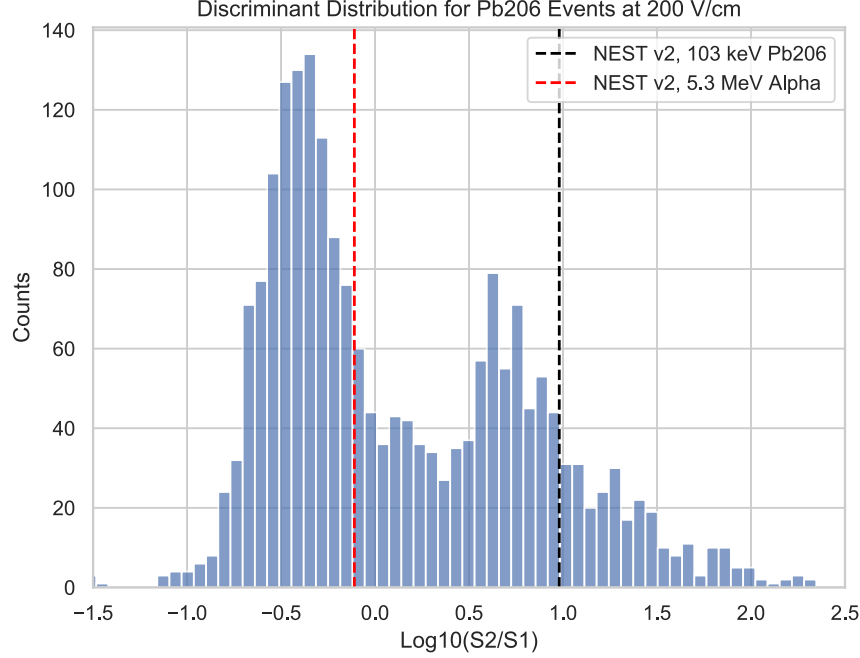


Figure 7.22: Distribution of discriminant ($\log_{10}(S2/S1)$) for observed ^{206}Pb events with NEST v2 predictions for α and ^{206}Pb recoils shown as red and black dotted lines, respectively.

From Fig. 7.20 and Fig. 7.21, it is clear that our observations are not well modeled by a mono-energetic ^{206}Pb nuclear recoil in NEST; for a 103 keV ^{206}Pb ion at 200 V/cm, NEST predicts mean yields of $n_{\text{ph}} \sim 1000$ photons and $n_e \sim 150$ electrons, which differs significantly from our measured yields. However, this is somewhat expected, as there are a number of effects which alter the signal spectrum of the heavy ion:

1. Energy straggling and partial energy deposition in the LXe, resulting in a smeared energy distribution (which depends on the ion and the surface properties of the source).
2. Charge loss, which leads to further imbalance between the S1 and S2 signals and systematically lowers the nuclear recoil band/discriminant.

It is possible that due to such effects, the NEST prediction shown for a mono-energetic ^{206}Pb recoil serves as an S1 endpoint of our observed ^{206}Pb band. Since the S1 and S2 yields are peaked at values which highly disagree with the NEST predictions, a non-trivial combination of surface effects is needed to reconcile these observations with the model. Furthermore, based on our GEANT simulations discussed in Sec. 6.2, the source layer would have to be much thicker than expected in order to smear the ^{206}Pb energy distribution into a uniform one. Additional work will therefore be needed to compare these observations with NEST and incorporate our data into the existing heavy ion model.

Regardless of the microphysics implications, we still have an impactful result with respect to WIMP search analyses. In LUX and LZ, such ^{206}Pb backgrounds are of concern primarily as a surface background at the detector walls, where they are likely to experience comparable light collection and surface effects. Given that we took care in DAX to minimize the thickness of the source layer and positioned the source in the fiducial center of our detector, it is difficult to devise a situation where these backgrounds can be more appropriately characterized.

We can directly compare our ^{206}Pb events with WIMP search data from Run 3 of LUX [13][16]. Furthermore, our drift field of 200 V/cm is similar to that used in Run 3 of LUX (180 ± 20 V/cm). However, in order to do a fair comparison using measured S1 and S2 yields, we scale our ^{206}Pb data by applying the ratio of g_1 and g_2 parameters appropriately:

$$S1_{\text{LUX}} = S1 \frac{g_{1,\text{LUX}}}{g_1}, \quad S2_{\text{LUX}} = S2 \frac{g_{2,\text{LUX}}}{g_2}$$

This is equivalent to directly comparing the quanta produced at the interaction site. We will refer to these quantities as our “LUX-adjusted” S1 and S2.

In Fig. 7.23, we overlay our adjusted ^{206}Pb events (red circles) on LUX data (black) in $(\log_{10}(S1), \log_{10}(S2))$ space. The LUX calibration ER (blue) and NR (red) bands are shown. The observed ^{206}Pb events overlap with the NR band in the low-energy search region, and below the NR mean across a wide S1 range. The plot also contains LUX events removed by fiducialization (faint grey dots); our observed ^{206}Pb events overlap well with those that are below the NR mean, which are reported to be likely surface backgrounds.

Even at the center of the fiducial volume, with charge loss and field non-uniformities mitigated by design, a surface ^{206}Pb source characteristically imposes itself on the WIMP search region. Increased charge loss would lower the recoil band further, so this measurement may actually serve as an upper bound for cases of surface contamination. It is clearly critical for dark matter searches to minimize such sources of contamination; position reconstruction error for these small S2 signals and field non-uniformities near the walls will only worsen background leakage into the fiducial volume and compound peripheral uncertainties. However, given the technical limitations of minimizing such contamination, it is critical to build accurate background models of such recoils to derive a realistic expectation for backgrounds in the WIMP search region.

Figure 7.23: Observed ^{206}Pb events (red circles) overlaid with LUX WIMP-search data [16] (black) and LUX ER (blue) and NR (red) calibration bands. Grey points (bottom) are events observed outside the LUX fiducial volume.

Chapter 8

Conclusions

“Begin at the beginning,” the King said gravely, “and go on till you come to the end: then stop.”

— Lewis Carroll, *Alice in Wonderland*

While xenon detectors have still not claimed discovery of WIMP dark matter, they have shown extraordinary sensitivity and discovery potential. We are approaching an age of massive, multi-tonne detectors such as LZ, which attempt to either discover DM particles or push exclusion limits for the spin-independent WIMP-nucleon cross section down to 10^{-48} cm², near the threshold for neutrino coherent scattering. In this sense, these next generation Xe experiments may exhaust a sizeable portion of discoverable WIMP phase space and ultimately usher in a new era of dark matter detection.

Neutrino backgrounds aside, there are a number of known complexities that must be addressed to optimize these massive Xe detectors. Effects in the periphery of the detector that worsen background leakage, shrink the fiducial volume, and increase uncertainties must be studied thoroughly to maximize sensitivity. In this work, we studied important peripheral dynamics that affect Xe detectors, using the LUX experiment as an important case study.

Prior to the LUX Run 4 WIMP search, a grid conditioning campaign induced significant charge in the PTFE walls of the detector, resulting in large field non-uniformities in the active region. This caused a number of unexpected complications, including entangled signal and position reconstruction errors. We showed that despite an evolving, asymmet-

ric charge distribution across the detector walls and a non-trivial detector geometry, it is possible to map erroneous reconstructed variables to “real space” variables by using layered interpolation techniques, electric field models, and spatially uniform calibration data. We presented “Jacob’s Position Mapping” (JPM) algorithm, which performs bijective, time-dependent mappings across the entirety of Run 4 data to allow for studies of backgrounds, fiducialization, and electric field effects.

Severe electric field non-uniformities can be challenging to characterize, but even they can be corrected for in analysis. Radioactive contamination of detector materials, on the other hand, is practically impossible to avoid at the levels required for next generation experiments. We need dedicated setups to measure and constrain backgrounds resulting from such contamination, so as to minimize errors in our background models and properly account for WIMP-like events. For this reason, we designed and built a small R&D detector in the DAX xenon testbed system at UC Davis to study perhaps one of the most important “wall backgrounds”: ^{206}Pb , which results from the α -decay of ^{210}Po .

In order to measure this nuclear recoil in LXe, we established multiple techniques for implementing ^{210}Po sources in the DAX dual-phase TPC. The first technique uses α -triggering with a PIN diode and custom readout circuit, with the diode source immersed in the LXe. The other technique involves the creation of spatially localized rod sources, with a thin (1–10 nm) source layer to minimize charge loss and energy smearing of the ^{206}Pb nucleus. Both techniques utilize a novel chemical deposition procedure for adhering liquid radioactive sources to glassy or metallic surfaces, and may be more broadly applied for characterization of other interesting particle sources in xenon.

By implementing a custom ^{210}Po source in the DAX TPC, we were able to isolate samples of ^{206}Pb events and characterize their response in LXe. We found that even with careful mitigation of surface effects, the observed ^{206}Pb events form a nuclear recoil band with S1 yields up to an endpoint of ~ 1000 photons. When comparing our observed ^{206}Pb events with the ER and NR bands of the LUX experiment, we found significant overlap with the low-energy WIMP search region of the nuclear recoil band, providing direct evidence that ^{206}Pb

events are likely a significant component of background contamination and could explain excess events observed.

This result speaks to the significance of measuring and modeling such backgrounds. Ideally, we would like to use our observations of ^{206}Pb to inform xenon microphysics models, which are ultimately used to build detector-specific background models. In this thesis, we discussed the development of NEST v2, the latest noble element simulation package, as well as the current form of its heavy nuclear recoil models (which have not yet incorporated our recent ^{206}Pb measurements). While we presented NEST v2 predictions for a mono-energetic 103 keV ^{206}Pb nucleus, we are unable to directly compare our DAX ^{206}Pb measurements with NEST at this time, since there are uncertainties in the energy distribution and charge loss of the nuclei which depend on the surface properties of the source. More work will be needed to incorporate the ^{206}Pb data into the NEST models; perhaps a simultaneous fit of existing wall background data with our ^{206}Pb measurements would allow us to parameterize the challenging surface effects.

There are some exciting applications for this method of characterizing sources in Xe. As previously mentioned, we may apply the same source-creation techniques to other particles of interest, such as low-energy β /X-rays, positrons, or other important nuclear decay chain daughters. Dedicated measurements of these sources in xenon detectors would facilitate the development of a suite of precise models for the NEST simulation package. Not only would this better constrain future background models for a variety of radioactive contaminants, but may ultimately lead to a deeper understanding of the microphysics, and perhaps even a first-principles physics model which fully captures the underlying nuclear processes.

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