Fiat LZ: Design and Light Simulation in the Next Generation of Dark Matter Detectors

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April 30, 2015

Abstract: In order to prepare for the LZ dark matter detector currently being built, I designed PTFE elements for front and back reflectors in the detecting volume to help increase light collection to the photomultiplier tubes. I also simulated the effects of various different reflectors in order to assess what would most amplify photon collection, accounting for differences in geometry and reflectivity. I found that the thinnest reflectors possible would most increase light collection because they least affected the path length of photons and lowered their chance of being absorbed by the liquid xenon.

I. Introduction

Searches for the direct detection of dark matter are underway across the globe. Though no specific project has given a reliable signal, they continue to seek out different candidate particles at different masses, but the most likely answer to the dark matter conundrum is the Weakly Interacting Massive Particle, which should appear at masses in the range of 1-3000 GeV. Currently, the Large Underground Xenon (LUX) experiment sits among the most sensitive dark matter detectors, but it hasn't yet encountered a reliable WIMP signal, and research groups around the world are making plans for its successor. A joint task between the LUX and ZEPLIN collaborations, the LUX-ZEPLIN (LZ) experiment promises greater sensitivity than its predecessors by increasing the bulk mass of the liquid xenon used (7 metric tons vs. 370 kg) as well as by limiting the background of particles that bombards the surface of the earth; the apparatus should be so quiet and noiseless that only dark matter particles and neutrinos can make to the inner fiducial region of the detector, resulting in a clear signal that as of yet has not been detected.

The xenon detector functions as follows. Particle interactions with the liquid xenon create photons at a specific wavelength (175 nm) as well as electrons. The initial photon flash functions as the first signal called S1. The electrons then drift upwards in the xenon because of an applied electric field within the detector. When they encounter an even stronger electric field at the top of the detector, they produce photons, creating the S2 signal. The time between these signals, along with seeing which photomultiplier tubes observed the photons, help researchers locate where in the tank the event took place. Most importantly, the ratio between S1 pulse height and S2 pulse height has an important correlation with what kind of recoil interaction, electron or nuclear, occurred with the xenon. WIMPs are hypothesized to have only nuclear recoils and,

because of their incredibly small cross-section, they are expected to interact only once in the detector, while neutrons entering the detector produce a very similar single interaction profile but are likely to interact many times in the detector. By discriminating by pulse shape and S2/S1 ratio as well as seeing how many interactions occur in the detector by any given particle, tank detectors like LUX and LZ can find signals that could only be caused by WIMPs.

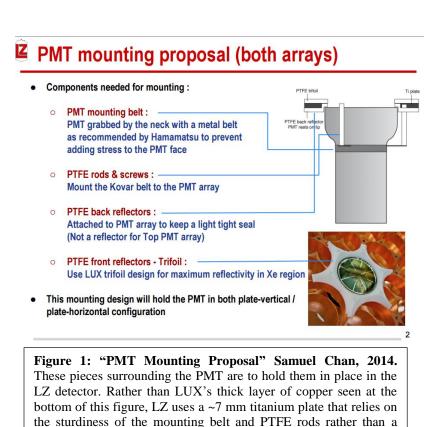
Currently, LZ is still being planned and assessed rather than built, but reliable, complex simulations that model its environment exist alongside the next generation of materials and components that will go into the body of the detector. Obviously, the quality control and further approval of the detector necessitates these designs and simulations.

My job was to work on both sides of this process of preparation: I designed parts of a testing apparatus that will be used in LZ itself and simulated those parts' material effects within the detector at large. More specifically, I designed the method by which photomultiplier tubes will be held and how light might be directed toward them; everything but the collecting surface in this design must be covered at the cryonic temperatures of the detector. The simulations, then, examined the consequences of certain variable dimensions of the designs I created, specifically how the parts affect photon collection in the photomultiplier tubes.

II. Design

On its face, my design work was an engineering challenge, but the physics underlying the materials and components involved merit attention. LZ requires PMTs different from those in LZ, though the geometries of the two systems are similar. Different parts will be necessary in both placing the PMTs inside of LZ and in housing them for testing and study. The tubes, made by Hamamatsu, have collections surfaces three inches in diameter, while the ones in LUX are two-inch models. Geometrically, they narrow from this width to a narrower cylindrical body.

Whatever their arrangement in whatever apparatus, they must be held in place, and all surfaces, apart from the photon collection surfaces must be covered with a reflective material, in this case Teflon. Teflon has the surprising quality in liquid xenon of having a high reflectivity (.95-.97) at the 175 nm wavelength of scintillating photons. Reflecting the photons increases the chance of collection by the PMTs, but it also increases the path length and likelihood of absorption by the xenon. (The average path length established for photons before absorption in simulation is 8.6 m, which is a conservative estimate.)



The differences in PMT arrangement and specifications will also affect how hits are registered inside of LZ. Particles are traceable in three dimensions as they pass through the

substantially larger piece of metal.

detector by measuring the shapes in signals and the order of PMTs activated; altered geometries will mean that an event in LZ aren't exact copies of those in LUX, even if scaled to the right size.

Additionally, the parts used to house the PMTs must be made of specific materials with interesting properties. Any metals used must be free of any unstable isotopes that might decay and create noise in the detector, thereby washing out possible WIMP signals. In fact, the largest source of noise is found in the radioactive isotopes that comprise parts of certain wires and electronics. The collaboration has settled upon steel that has been carefully prepared to be without cobalt. (The latter contributes radioactively through the cobalt-60 isotope.) The alloy Kovar, made largely of iron, cobalt, and nickel, had been used in the past, but the cobalt-free steel formulation has been declared more suitable for LZ.

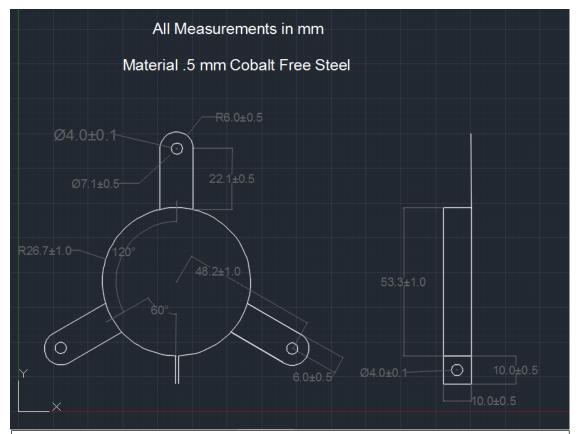


Figure 2: Mounting Belt for PMTs, Max Genecov, 2014. This belt is to be wrung around the neck of the PMT and held in place both by a PTFE bolt around it and by the PTFE rods that suspend it from the other PTFE pieces and the titanium housing plate.

The reflectivity of metals, however, doesn't factor into the discussion, because the only surfaces visible inside of the detector must be made of PTFE, also known as Telfon when branded. These parts must be fitted carefully around the PMTs and the sleeves that hold them. This is largely a best fit process, limited by the specifications of the PMTs and the testing apparatus in general.

Ideally, one would use a huge sheet of Teflon with holes punched in it to cover the base of two collecting surfaces in LZ. However, this technique would have to account how Teflon shrinks at lower temperatures. Since xenon's boiling point is 165 K and LZ must operate very close to that temperature to keep the xenon in its proper state, it is difficult to make precise cuts in the Teflon as well as predictions about how the sheet will shrink.¹

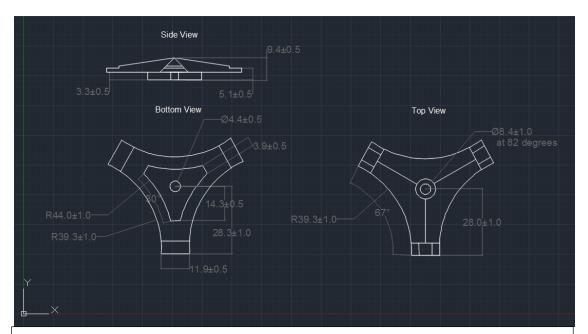


Figure 3: Trifoil Reflector Components, Max Genecov, 2014. This piece only represents half of the trifoils. The other half has arms that extend beyond the edges of the reflector in order to interleave themselves with the slots on these trifoils. Like in woodworking, this method creates a firmer, light-tight seal than simply abutting the trifoils.

¹ The thermal coefficient of Teflon is 1.12-1.25e-4 K⁻¹. This means that the Teflon will shrink by a factor of 1.5-2% when submerged in the cryonic temperatures that will be used. Meanwhile, titanium has a coefficient of 8.6e-6 K⁻¹, obviously much lower. The Teflon would shrink in some unpredictable direction if there were simply a sheet of it, rather than slightly and radially in this trifoil design.

To compensate for this shrinkage, I designed a system of interlocking trifoil parts like those seen in Fig. 3. These parts would shrink radially and predictably while still fitting together. More importantly, they would be easily constructible for different sizes and arrangements of PMTs. Though only one is displayed above, there are two models for the trifoils. The ends dovetail into each other, providing an easy and flush fit. Finally, the Brown Machine Shop was able to make some proof-of-concept pieces of the trifoils fitting together, though these pieces are connected to other parts.

Under the trifoil will appear a metal plate with holes made for the PMTs and the bolts that hold them in place. Under this, though, there would be a back reflector, seen below, that would ensure the light-tightness of the inner chamber of the detector.

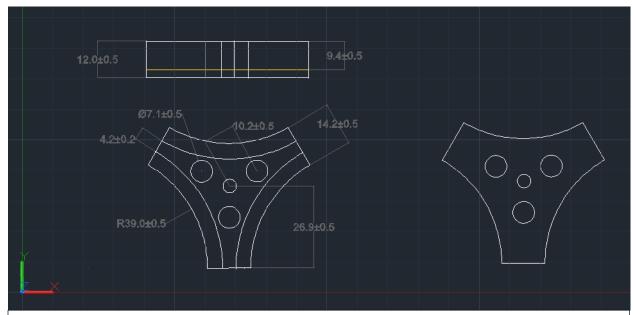


Figure 4: Back Reflector, Max Genecov, 2014. These back reflectors might be difficult to visualize in three dimensions from these drawings, but they are made to be recessed inverted versions of the titanium plate that they surround. They help keep the PTFE rods in line as well.

As one may be able to see in Fig. 4, this back reflector swaddles the metal plate (the edge marked in the side view by a yellow line) and comes up flush to meet the bottom of the trifoil. No metal is exposed to the detector, only glass and Teflon.

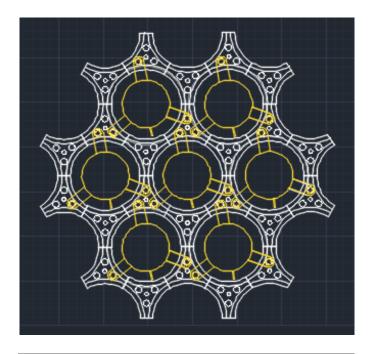


Figure 5: Connected Trifoils with Bolt Alignment, Max Genecov, 2014. My designs line up nicely to form this "honeycomb" design as I have named it. These seven PMT banks are to be built as a testing rig for the PMTs before they head to Sanford Lab.

The overall picture of these parts, placed among PMTs looks like a honeycomb as seen in Fig. 5. It could be expanded to any number of PMTs arranged in a regular hexagon. The edge pieces cause a problem in that they poke out on the edges, but a trifoil with an arm cut off would be an easy alternative. The diameter of this design barely fits within the parameters that those who will be using the apparatus desire, but, given the necessities of the plate and the PMTs, this is the most compact design I could muster.

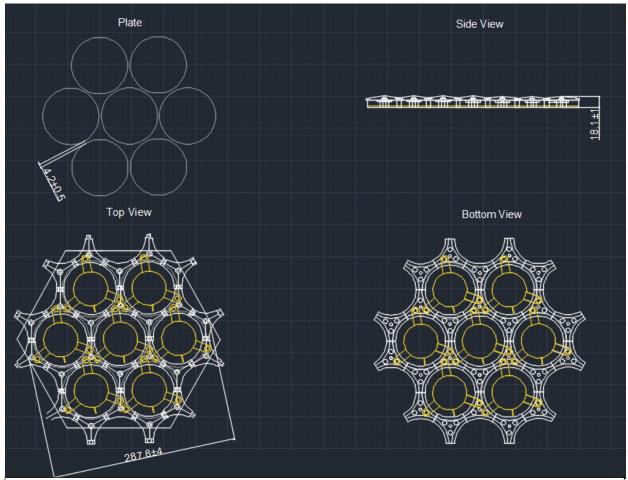


Figure 6: Views and Measurements of the Honeycomb Max Genecov, 2014. If we were to shave off the edges of the reflectors that jut outside of the hexagon drawn over the top view of the honeycomb, we would have an apparatus that is at its widest point 288 mm, which is just under the 12-inch maximum we established for the testing apparatus.

III. Simulations

Though the trifoils must be designed carefully in two dimensions, the vertical component in the detector is a free variable. One might expect a taller trifoil to reflect more photons onto the collection surface. However, because Teflon reflects light diffusely rather than specularly, it isn't a trivial calculation to find where photons at various heights will end up. Therefore, I simulated photons originating at multiple heights using different reflector geometries.

Additionally, the existing simulation geometries included a simplified model for the trifoils: a sheet of Teflon with frustums cut into it. Though the difference was slight, it seemed

worthwhile to make the trifoils more pointed at the tops to resemble my designs. Though this effect wouldn't be visible at large distances, I hypothesized that the greater surface area of the canted sides might increase light collection.

Though we had a clear line of sight to the goal for this project, the path was fraught with unforeseen programming difficulties. Old versions of simulation and conversion codes masqueraded as new ones. Errors written into early versions of the simulation were left untended until I had to deal with them. Miscommunication within files abounded. These problems ramped up in difficulty from most trivial to fundamentally challenging in roughly chronological order.

To begin, we were using a code called LUXSim that simulated various environments from the LUX tank to LZ to toy models of such systems. Hosts of programmers from across the LUX collaboration had built the simulations in C++ on the skeleton of the particle physics modelling package GEANT4 for the past six years. Once I was able to get LUXSim up and running, I was able to follow single particles, from photons to alpha nuclei to things much more exotic, travel through the liquid xenon with specific energy, direction, and position. I could also set off one hundred thousand instances of such particles to establish large number statistics within the environment.

I used the LUX geometry for my work because the reflector height seemed to be written as a variable in one of the files. I later learned that this value was being ignored in a different geometry file, instead holding a hard-coded measurement for it—the standard 0.668 cm—but that problem, once found, was remedied. I could toggle the value to whatever height I chose, within certain limits.

There are certain spaces in the geometry build codes of LUXSim that are clearly defined as bare planes or cylinders. When the newly elongated reflectors encounter these definitions,

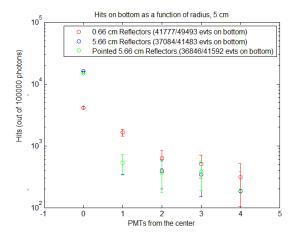
they compromise each other, creating a hole in the geometry. If a photon or any particle for that matter were to enter this space, there's a possibility that the simulation would register it as having left the whole environment and stopping viewing it. To avoid this problem, I raised the reflector height to 20.7 cm for a proof of concept and no more.

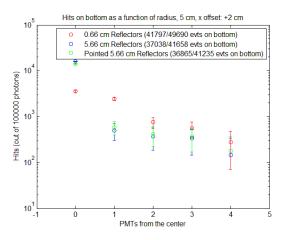
This all sounds well and good, but the simulations, when run, announced a different problem. After analyzing the data, I could see that the comparisons between original runs all looked wrong. These plots are all the result of the same test, only altering the geometry: I simulated 100,000 photons with random velocity vectors at 0, 3, 6, 9, 12, and 15 cm above the collecting surface of the central photomultiplier tube. I changed the height of the reflectors as well as the intensity of the slope of the sides of the trifoil to find what effect they might produce.

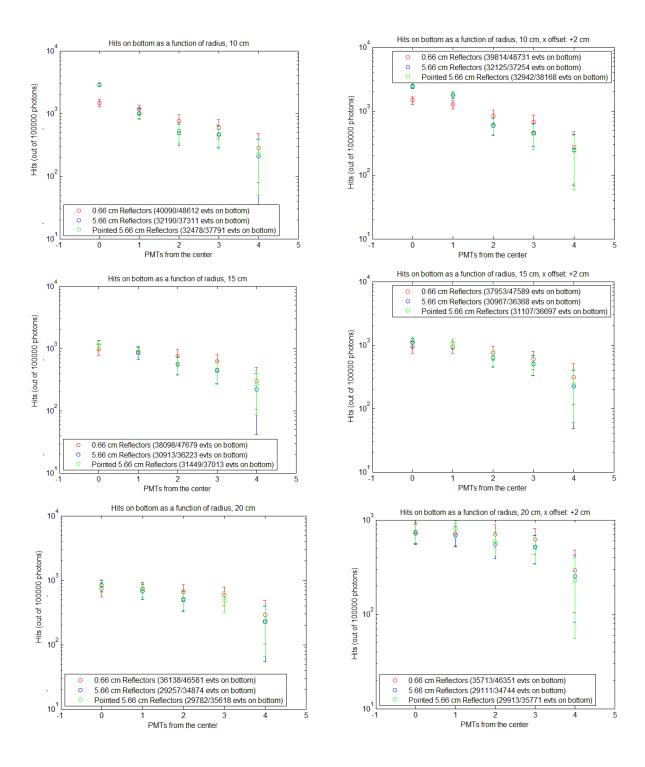
However, these tests uncovered faulty values hardcoded into some of the geometry files utilized in LUXSim as well as a host of other, personal mistakes. They created data that ignored the height of the reflector walls. Photons would pass through where the Teflon should have been, even in the 20.7 cm reflector case. Other plots featured interesting trends, but make little sense in terms of actual values. Different errors would crop up in different simulation runs until we were able to suss them all out individually. One type of problem would make the 5.7 cm reflectors case collect more light in every PMT. The fact that the 5.t cm reflectors' peak just below the height of the photons' origin leads one to predict that more photons would hit the center PMT in the higher reflector case, which they did in these runs. However, such an analysis would also predict fewer hits in the succeeding PMTs because of the relatively small solid angle that each succeeding reflector would occupy for the photons; even after bouncing off of these further reflectors in the off chance that the photons did reach them, the photon path length would grow, increasing the chance that the photons would be absorbed by the liquid xenon itself.

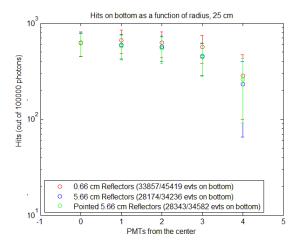
The cause of both of these problems is that some files were dependent on the reflector height I changed and others used the hardcoded 0.668 cm height by default. This resulted in situations where it seemed that photons would just pass through the Teflon unimpeded when in fact there was no Teflon there. Once the errors were painstakingly removed from the process, one by one as they became evident, I was able to make progress on reliable simulations.

To effect more realistic situations than the test cases I used to make sure that the geometry and physics were correct, I utilized similar initial conditions to those in the faulty simulations but at heights of 5, 10, 15, 20, and 25 cm. Additionally, I only used three different geometry cases for the reflectors: the standard 0.668 cm reflectors with flattened tops, taller 5.668 cm reflectors with flattened tops, and pointed 5.668 cm reflectors (to see if this altered angle and surface area visible to the photons would at all affect light collection). I also ran a test where the photon origin was 2 cm from the axis of the detector to examine whether the pointedness of the reflectors would affect collection. Another test switched from diffuse reflection to specular reflection in Teflon to see if that distinction might have affected our choice of hypothesized reflectors.









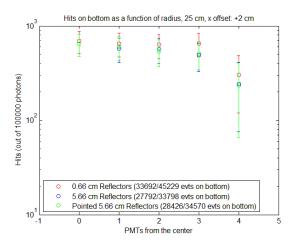


Figure 7: Comparing Centralized and Offset Photon Generation Along a Radial Selection of Five PMTs. There is no difference between light collection rates in the centralized and offset cases that is greater than the Poisson error of the number of events (+/- ~200 in each case). Therefore, we can reasonably assume that the reflection rates are constant within an xy plane and that the simulation is working. Additionally, and possibly more importantly for the general findings of this thesis, though there is a general amplification of central PMT collection in the 5.7 cm reflector case at 5 and 10 cm, the effect dies away at about 15 cm, and in every case, the shorter reflectors collect more photons overall, even if they don't do so in the central PMT. The pointed geometry, with its modest increase in collection, cannot make grounds on the loss generated from the change in height.

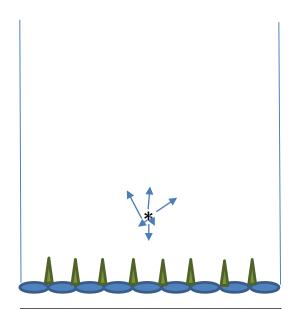
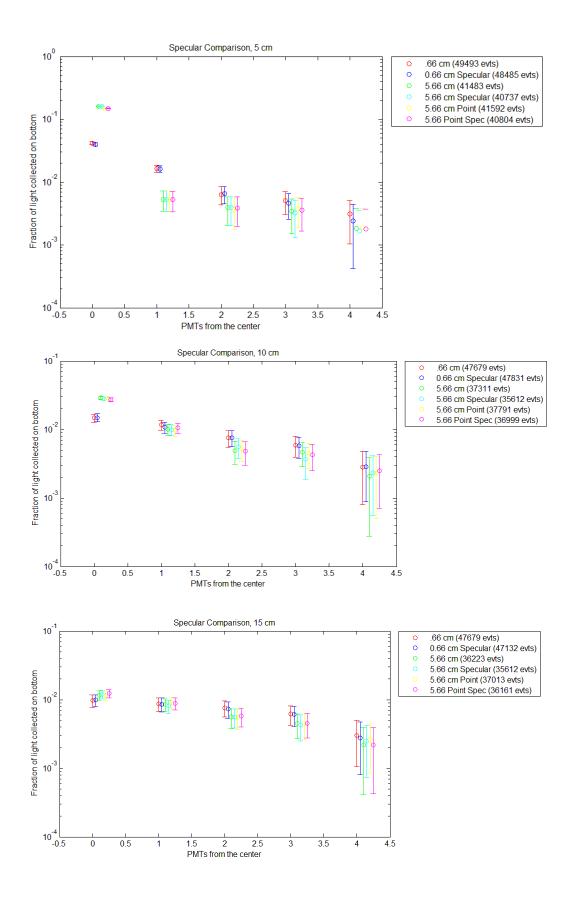


Figure 8: Cartoon Illustration of 5.7 cm Tall Reflector Case with Photon Generation at 15 cm. Here is a pedagogical illustration of what the simulation is actually doing. The photons are generated as travelling in all directions but originating above the central PMT. The central PMT and the PMTs to the right of it are the ones seen in Fig. 7.

Not only do the plots in Fig. 7 show no difference between the locations of the photon sources, but they also reveal that the higher reflectors direct fewer photons to the collection surfaces at each height. Even though it seems like the dramatic difference in hits at the central PMT would make up for the higher reflectors' lower counts in PMTs further out (the many more PMTs arranged radially outweigh the single central PMT here), the simulations show that even at close ranges the shorter reflectors collect more light. Additionally, the new pointed geometry I added did little to affect collection in one direction or another, at most a 1% increase; the height difference between reflectors washes out any tertiary effects or alternate collection mechanisms that it might have produced.

I saw the taller reflectors collect less light in the specular reflection case as well.

Though these instances collected very slightly less light on average than the natural diffuse reflection, they follow the same trend of depleted light in the tall reflector case as the other environments.



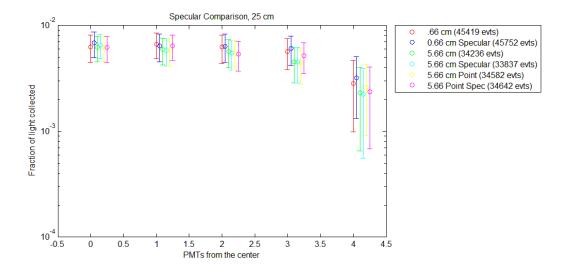
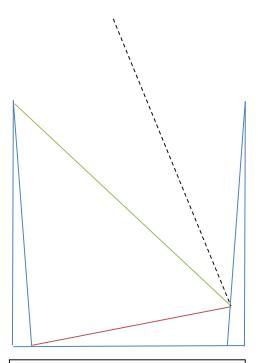


Figure 9: Comparison of Specular and Diffuse Reflection Cases with Different Reflectors at Various Heights. The differences between the specular and diffuse cases are remarkably insignificant, if they are even there at all and are not in fact effects of Poisson error. This leads one to wonder what the differences between diffuse and specular reflection there are at all in a detector where photons interact with different substances, reflective and redirecting, up to one hundred times before being absorbed or collected.

One might expect that the specular case would be more predictable than the diffuse case in terms of reflection angles and that that would lead an amplification in the number of events in the central PMT, but such an effect is not visible in Fig. 9.

I explain the results in both cases by saying that the 5.7 cm reflector regime, whether the teflon reflects light specularly or diffusely, increases the total path length of the photons, thereby increasing the possibility that they would get absorbed by the liquid xenon. When a photon encounters the teflon, it reflects in one direction or another; very few of these collisions would send the photon toward a collecting surface. Here is an explanatory diagram for a rough geometrical argument for the diffuse case:

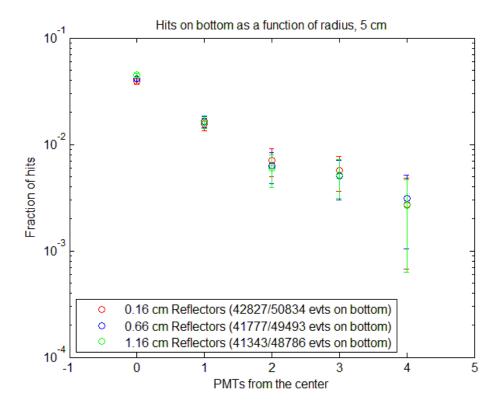


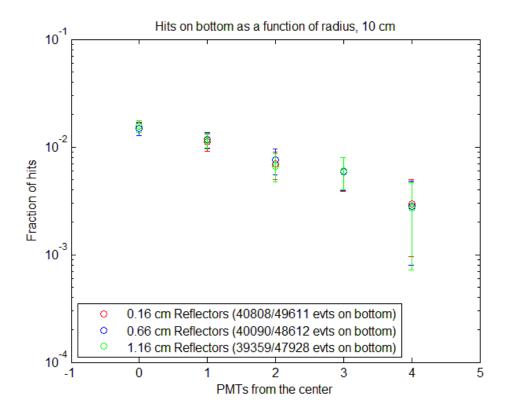
10: **Figure** Cartoon Reflection Pedagogy. Any photon that is reflected above the red line either encounters another reflector or escapes the reflector well. In either of those cases, (50-75% of the time if we guess that the reflection is isotropic) the photon's path length increases, as does the photon's chance of being absorbed by the liquid xenon. This chance increases, though trivially, if the reflection distribution is instead assumed to be cos^2, the more physically relevant result in terms of solid angle.

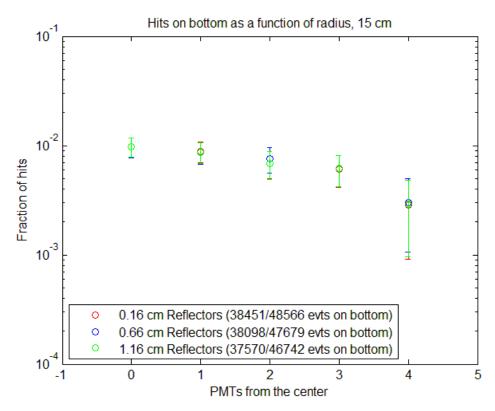
The incident photon (the dashed line) in Fig. 10 encounters the teflon reflector. It then has a possibility to reflect into the collecting surface (under the red line), hit the opposite reflector (between the green line and the red line) or bounce out of the reflector well into the body of the detector (above the green line) where it may be absorbed, hit another PMT or reflector, or Rayleigh scatter off of a xenon atom. The angle of the red line varies between 45 and 90 degrees, depending on where the photon hits the reflector. The chance that it hits the other reflector is always approximately 45 degrees. Therefore, there is between a 45 and 90 degree chance that the

photon exits the reflector well entirely. Whereas in the short, default reflector case, the photon would have sailed through the area unimpeded, heading toward another PMT, this 5.668 cm case demands a 50% to 75% chance for any given photon to increase its path length after encountering a reflector. This argument doesn't even take into account Rayleigh scattering at these lengths, which may occasionally occur within the well, thereby redirecting the photon in another, random direction that, because of the solid angle subtended by the collection surface, will likely reflect off the walls or escape the well entirely rather that get collected.

To investigate further, I ran tests on much shorter reflectors as seen in Fig. 11 below at the same benchmarks as the others. These runs show a ~2% increase in total light collection at each height for each successive drop in height with no corresponding change in the location of such collection, though to a leading order, these are all functionally the same plot in terms of rough value and distribution.







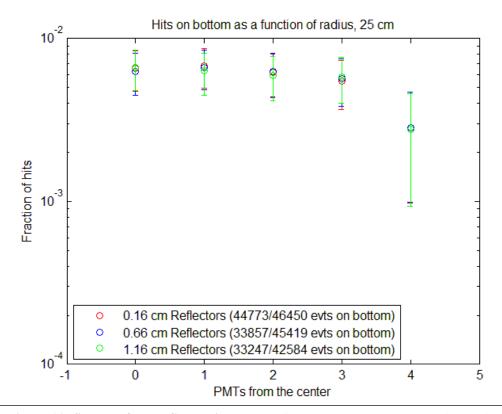


Figure 11: Short Reflector Comparison. Centralized photon generation at various heights with these shorter reflectors shows a very modest increase in the number of total photons collected as reflector height decreases, but an increase that, unlike the difference between the specular and diffuse cases, lies above the Poisson error.

IV. Conclusion

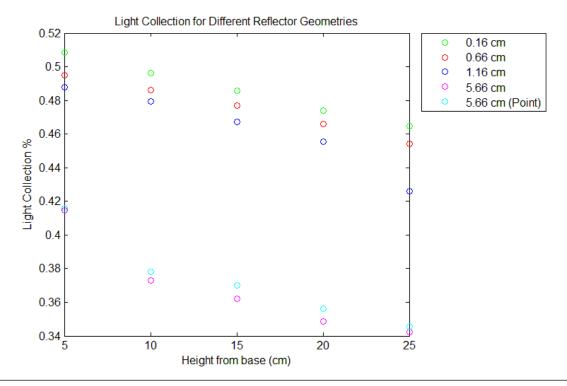


Figure 12: Light Collection Comparison. Here we see the compiled light collection rates of all of the reflector geometries compared. The slight improvement of the pointed design would be useful in Gamma-X event discrimination (discussed later) but would be a drop in the bucket compared to the more general loss of light collection (about 20%) compared to the short reflector cases.

Though the taller 5.7 cm reflectors showed a statistically significant peak in the central PMT's light collection fraction up to 15 cm above the collecting surface, they severely underperformed in light collection summed over all PMTs, as is summarized in Fig. 12. The geometric model I proposed earlier of photon's path lengths being extended seems to be the cause of these lower counts; photons bouncing off the reflectors in the 5.66 cm case would, in the shorter cases, continue through the xenon and likely hit a PMT's collecting surface. In fact, light collection improved measurably with each successive drop in reflector height so that the thinnest reflector possible would be preferential in the design of the LZ detector. The profiles of the smallest reflectors also have similar dropoff profiles, so the shortest reflectors' improvements

off of the default reflectors are comparable. Though a 2% improvement from the default trifoil geometry might not be actionable for the LZ engineers to alter the existing plans, they outperform the tall reflectors by >20% and the smallest reflectors may be considered for use for the sake of simplicity as well as efficiency, as long as they are opaque.

Additionally, a retooled geometry with a larger collecting surface very slightly improved collection (~1% increase) on the tall reflector tests but was negligible in the case of the shorter reflectors because the difference in solid angle coverage at heights within the fiducial volume of the detector (>5 cm) was so small. They would also be harder and more expensive to machine, so And so, thin, flattened versions of my trifoils would allow the most photons to be collected by the PMTs.

The difference between specular and diffuse reflection may have guided misconceptions about how the tall reflectors might have been more successful collecting light, but even these misconceptions could be mistakes at their very core. Whereas the diffuse case has a random velocity vector and a random reflection angle, the specular case only has the random velocity vector. Because the reflector is neither an infinite length case (the proportions of photons heading in either direction, up or down, along an infinite cylindrical reflector well should be equal) nor a "semi-infinite" case (where the photons would be allowed to die in the well, therefore extinquishing most of the random walk, diffused photons), the difference in the cases is harder to see. What it seems to be is that a significant number of diffused photons that would, in the specular case, just have been bounced out of the well are instead redirected into the PMT. In the case of the shorter PMTs, it is very likely that the slightly lower counts seen in the specular case have to do with the shallowness of the angles of the trifoils heading into the PMT.

There is one case where the taller reflectors might be useful, illustrated in Fig. 12. If a particle interacts twice within the detector and one of these interactions takes place near the PMTs, out of the electric field of the fiducial volume, it will not be detected properly. By having such deep PMT wells, these events would happen less often; they could only access the area outside of the fiducial volume if they travel within the small cone created by the well and do not bounce off the reflectors. These events, called Gamma-X events, have unusual signals that can confuse the normalized energies and pulse shapes of electron and nuclear recoils. Though it would be a boon to attenuate Gamma-X events, one would have to reconcile that with having 75% light collection of the shortest reflectors.

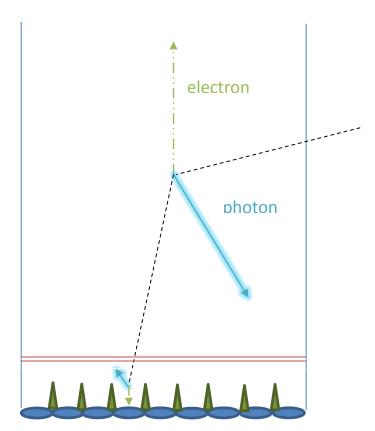


Figure 13: Gamma-X Event Illustration. A particle can interact twice while passing through the detector. Gamma-X is the name where the first interaction is entirely normal, but the second takes place under the cathode grid (burnt orange parallel lines). Under the burnt orange lines, the electric field is reverse so that electrons cannot drift upward in the fiducial volume of the detector and create S2 events. These cause problems when trying to calculate the S2/S1 value and muddle the difference between nuclear and electron recoils. Tall reflectors would discriminate against these events because they would happen so close to the PMT collection surface that the photons would be collimated and thereby isolated and visible as Gamma-X events.

Previous conventional thought from the LUX group conflicts with my simulations. These assumptions led previous design throughout the process of designing and operating LUX and LUX parts. Now that we further understand how diffuse reflection acts upon the Teflon, we can say that these assumptions that led to the canted angles of the trifoils and their height are both unnecessary and faulty. What would be best for the trifoils in LZ, it seems, is a series of flat plates that interleave at the edges so that none of the titanium plate is visible to the photons.

Though my conclusions are opposed to conventional thought, it doesn't seem to conflict with any previous simulations. They can be accommodated without much theoretical pushback both in how the detector will be built and how Teflon reflection of photons functions in the detector. There is, however, a forthcoming, comprehensive simulation from the LZ group (Jeremy Mock, 2015) that will hopefully include a clarification as to my results about the reflectivity of teflon.

Acknowledgements

Richard Gaitskell, Simon Fiorucci, Samuel Chan, Will Taylor, James Verbus, Vic Gehman, Dongqing Huang