Simulating neutron absorption in ^{136}Xe

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Abstract

A method for simulating the distance and time it takes neutrons to be absorbed in liquid ^{136}Xe is presented. We then improve upon this method by varying the scattering angle, adding a thermal walk, and considering the effects of nuclear resonances. Our results show that for a neutron of a given initial energy, the displacement and time for absorption are given by a range of values and it is therefore difficult to predict exactly when and where a neutron will become absorbed in ^{136}Xe. A range of displacements and times for absorption in ^{136}Xe are determined for neutrons with initial energies ranging from 50 MeV to $\frac{1}{40}$ eV. These ranges will used in the nEXO experiment to improve the experiments accuracy in observing neutron less double beta decay.

1 Introduction

Over the past few decades many observations made by astronomers, such as the velocity at which galaxies rotate [1], suggest that there is much more mass in the universe than once thought. These galaxies are rotating much too fast and should be falling apart because the gravitational force is not strong enough to keep the matter in the galaxy bound. The only explanation is that there is much more matter in these galaxies than we once thought. This so-called dark matter cannot be detected through traditional observational astronomy, which uses electromagnetic radiation to observe celestial bodies.

It has been hypothesized that this extra matter takes the form of Weakly Interacting Massive Particles (WIMPs) [2]. WIMPs only interact through the weak nuclear force and gravity, and therefore cannot be detected through electromagnetic radiation. If the mass of WIMP particles is significant, then their mass could explain the observed dark matter.

One weakly interacting particle is the neutrino. The neutrino has no charge and was theorized to have no mass. Recent studies have shown [3] through neutrino oscillations that the neutrino indeed does have a small amount of mass. There is now an effort to accurately determine the mass of the neutrino. Knowing the mass of the neutrino would allow physicists to determine if the dark matter needed for galaxies to stay intact is coming from WIMPs. If WIMPs accounts for the dark matter then we can be confident in our understanding of gravity. If the mass of the WIMPs is too small and does not explain dark matter then we must re-think our understanding of gravity or our observation of the mass in galaxies is incorrect.

The nEXO [4] experiment is attempting to determine the mass of the neutrino by observing the rare neutrino-less double beta decay ($0\nu\beta\beta$). This decay is very hard to observe because only a few

isotopes are predicted to be able to undergo this decay channel [5].

There are many sources of background for the nEXO experiment such as muon-induced neutrons, radiation from materials within the detector, and alpha radiation from the sun. Neutrons that are created from solar muons can be a particularly troublesome source of background because these neutrons can be absorbed within the detector and excite the ^{136}Xe. The ^{136}Xe then becomes ^{137}Xe, which undergoes a β decay, whose energy spectrum overlaps with the $0\nu\beta\beta$ decay energy spectrum. This neutron-induced β decay therefore could then be mistaken for the $0\nu\beta\beta$ decay. It is therefore important to exclude data coming from this β decay.

To exclude this data we must know where and when these muon-induced neutrons will be absorbed. A neutron is typically absorbed once it has reached thermal energies ($\frac{1}{40}$ eV). Our goal is to track the neutrons as they traverse ^{136}Xe and reach thermal energies.

2 Methods

We have created simulations to determine the mean distance and time neutrons travel in ^{136}Xe before being absorbed. We then developed three new more realistic simulations by building upon the original simulation. Each of the simulations' outputs have been compared to determine how each improvement affected the distance and time it took for neutrons to become absorbed.

For simplicity, the original simulation, (which will from here on be referred to as ORIGIN), uses the assumption that all neutrons scatter at a constant angle. It also ignores the fact that once a neutron becomes thermalized, the neutron travels some distance before being absorbed. In addition it also ignores all nuclear resonances.

The first improved simulation, (which will from here on be referred to as AVARIETY) , improves ORIGIN by allowing a neutron scattering angle that is not constant, but given by a distribution of angles.

The second improved simulation, (which will from here on be referred to as WALKER) , improves on AVARIETY by allowing the neutron, once thermal, to undergo a random walk before becoming absorbed.

The third and final improved simulation, (which will from here on be referred to as RESONANCE) , improves upon WALKER by considering nuclear resonance data, such that if a neutron of a given energy collides with the ^{136}Xe and the neutron energy matches that of a nuclear resonance, the neutron is absorbed immediately.

2.1 Mathematical Methods

To determine the mean displacement of a neutron once it is absorbed, we use a statistical method which relies on the fact that a neutron will travel one mean free path on average before colliding with an atom. When a neutron collides with an atom it loses some energy and scatters at a given angle.

When a neutron traverses a substance, it can be thought of as entering a cylinder, shown in Fig. 1, containing many atoms of the substance. The neutron collides with these atoms as it passes through the cylinder. The average distance through which the neutron travels in this cylinder before colliding with an atom is called its mean free path λ given by [6]

$$\lambda = \frac{1}{N\sigma(E)} \tag{1}$$

where N is the number of atoms per volume of the substance and $\sigma(E)$ is the total cross section of the target atom at the neutron energy E.

The total cross section σ is dependent upon the substance the neutron collides with and is a function of the neutron energy. In order to determine the cross section for ^{136}Xe at any energy, we use a nuclear simulation package TALYS [7]. TALYS produces very accurate cross section data for energies above 1 keV. Below 1 keV, TALYS assumes the cross section is proportional to $\frac{1}{v}$ where v is the velocity of the neutron. This approximation is valid for some substances, but not for ^{136}Xe.

In order to determine the cross section for neutron energies below 1keV we use the CENDL database [8]. Combining data from TALYS and CENDL, we create functional fits that allowed an accurate determination of the cross section at any energy from 50 MeV to 1/40 eV. Knowing the cross section at any energy then allows us to calculate the mean free path for any energy using Eq. (1) .

After traveling on average one mean free path the neutron collides with the ^{136}Xe. In our simulations we make the assumption that every neutron travels exactly one mean free path and then immediately collides with an atom.

This collision can be modeled as an elastic collision of two spheres. If it is assumed the ^{136}Xe is at rest before the collision, a neutron will lose a fraction of its energy given by

$$\frac{KE_{after}}{KE_{before}} = \frac{m_n^2 + m_{^{136}Xe}^2 + 2m_1 m_{^{136}Xe}\cos\theta}{(m_n + m_{^{136}Xe})^2} \quad (2)$$

where m_n is the mass of the neutron, $m_{^{136}Xe}$ is the mass of ^{136}Xe and θ is the scattering angle. From Eq. (2) the energy after any collision can be calculated by knowing the initial energy of the neutron, the mass of ^{136}Xe, the mass of a neutron, and the scattering angle.

In Ref. [6] it is shown that the average cosine of the scattering angle for a neutron is given by

$$\langle cos(\theta^{k-l})\rangle = \langle \mu^{k-j}\rangle = \frac{2}{3A} \quad (3)$$

where A is the atomic mass of the substance the neuron is in, the k and l indices reflect that the angle we are referring to is the angle between the position vectors of the neutron at the k and l position which are the positions before and after the collision. For ^{136}Xe this corresponds to a scattering angle of roughly 89^o.

We use the assumption that the scattering angle does not effect the energy lost in a collision. Using this assumption and Eq. (2), we find that 2% of the neutron energy is lost in each collision.

Of course in reality there is a relationship between the scattering angle and the energy lost in a collision as you can see from Eq. (2). Our assumption that there is no angle dependence is valid for a neutron scattering off ^{136}Xe as long as the scattering angle is constant or almost constant, which is the case for our simulations. If the angle is varied more than 10^o, from Eq. (2) we see the fractional energy loss will only change to 1% of the neutron's initial energy. Therefore our assumption that the neutron always loses 2% of its energy in every collision is valid as long as we do not vary the scattering angle more than 10^o.

With our cross sectional fit, the scattering angle, and the energy lost in each collision, the mean displacement, which is derived in [6], can be determined by

$$\langle|\vec{R}|\rangle^2 = 2[\sum_{j=1}^{N}\lambda_j^2 + \sum_{j=1}^{N-1}\lambda_j \sum_{k=j+1}^{N}\lambda_k \mu^{k-j}] \quad (4)$$

where $\langle|\vec{R}|\rangle^2$ is the average square of the mean displacement of the neutron, λ_j is the mean free path for the neutron at a particular energy step j, and μ^{k-j} is the cosine of scattering angle between the k and j energy step from Eq. (3).

To determine the time it takes for a neutron to be absorbed by ^{136}Xe we need to determine the neutron velocity while it traverses each mean free path. The classical relation between energy and velocity may be used because $v_{neutron} \ll c$ for the neutrons in the energy range we are considering. Once the velocity and mean free path are determined for a given energy, the average time the neutron spends at that energy can be determined by

$$\langle \Delta t_j \rangle = \frac{v_j}{\lambda_j} \tag{5}$$

where v_j is the velocity of the neutron after the j^{th} collision and λ_j is the mean free path after the j^{th} collision. Therefore the total time for absorption, T is given by

$$T = \sum_{j=1}^{N} \Delta t_j \tag{6}$$

2.2 ORIGIN, AVARIETY, WALKER, RESONANCE

In ORIGIN, we assumed that the scattering angle was a constant given by Eq. (3). It was also assumed that the neutron was absorbed immediately after becoming thermal, and nuclear resonances were ignored.

In AVARIETY, the scattering angle was given some variance but the average was still given by Eq. (3). As neutrons slow down they no longer have the tendency to scatter forward as they do at high energies. To describe this behavior a normal distribution of possible scattering angles was used with a standard deviation of 5^o when the neutron was above 1 keV. This standard deviation was increased to 10^o when the neutron energy was below 1 keV. Then once the neutron reaches thermal energies, it is immediately absorbed. Also nuclear resonances of ^{136}Xe were ignored.

In WALKER, the neutron is not absorbed immediately after becoming thermal. Instead the neutron is allowed to undergo a thermal random walk before being absorbed. A thermal random walk is defined as the series of perfectly elastic collisions thermal neutrons undergo before being absorbed. Eqs. (1),(4),(5) and (6) are used to determine the displacement of the neutron while thermal and how much time is spent at thermal energies. Thermal neutrons are equally likely to scatter at any angle and so instead of Eq. (3) for the scattering angle a random distribution of angles is used. Also when the neutron is thermal it is in equilibrium with the ^{136}Xe and therefore no longer loses energy in collisions. This behavior is characteristic of a random walk.

To determine the number of collisions the thermal neutron undergoes before becoming absorbed in the WALKER simulation, the probability of absorption at thermal energies has been determined. For simplicity it is assumed that the only two reactions for a thermal neutron are elastic scattering and neutron absorption. With this assumption probability of absorption is given by

$$P(absorption) = \frac{\sigma_{absorption}}{\sigma_{absorption} + \sigma_{scattering}} \tag{7}$$

We have derived this equation by using the standard interpretation of a cross section which is that the cross section is proportional to the probability of a specific reaction occurring. Taking the limiting case shows that this is a reasonable measure of the probability of absorption. If the scattering cross

section goes to zero the probability of absorption is one, and if the scattering cross section goes to infinity the probability of absorption goes to zero.

In RESONANCE, the effects of nuclear absorption resonances in ^{136}Xe are taken into account. Nuclear resonances must be considered because high-energy neutrons may be absorbed by the target nucleus if the neutron energy matches that of a nuclear resonance. 32 resonance energies were considered from Ref. [8] and are shown in Fig. 2. Each resonance is given a width of 1% of the energy of that resonance. This width was determined by analyzing the averages width of the resonance peaks in Ref. [8]. In WALKER these resonances act as a filter such that if a neutron energy at any point hits a resonance energy, it is immediately absorbed.

2.3 Computational Methods

Using the functional fits of the cross section and Eq. (1)-(6) the mean displacement and time for absorption can be calculated. ORIGIN runs as follows:

1. Input: initial energy of neutron
2. Calculate λ from Eq. (1) $\Rightarrow$ store
3. Calculate v from classical relation $\Rightarrow$ store
4. Calculate t from Eq. (5) $\Rightarrow$ store
5. Calculate ΔKE from Eq. (2) $\Rightarrow$ store
6. Subtract Δ KE from neutron energy $\Rightarrow$ store as new initial energy
7. Repeat steps 1-6 until energy $<= \frac{1}{40}$eV
8. Calculate sums in Eq. (4) and Eq.(6)

AVARIETY, WALKER, and RESONANCE follow the same algorithm but with extra steps detailed below.

In AVARIETY step (8) is amended such that for every step j, an angle is picked from the distribution described in section 2.2. In WALKER, after step (7) the program continues to calculate the distance and time traveled while thermal. During each step of the thermal walk, the simulation decides if the neutron is absorbed or not by using the probability given by Eq. (7). In RESONANCE, after step (1) there is an extra step which checks to see if the neutron energy is that of a resonance energy, and if it is so, the neutron is immediacy absorbed.

3 Results and Discussion

A simulation was designed that determines the distance and time until neutrons, of different initial energies, are absorbed in ^{136}Xe. This simulation was then improved to include variations in the neutron scattering angle, the thermal walk neutrons undergo before becoming absorbed, and nuclear absorption resonances.

Fig. 3(a) and Fig. 3(b) show the results from ORIGIN, which assumes a constant scattering angle. Fig. 4(a) and Fig. 4(b) show the results from AVARIETY, which uses a variety of scattering angles. Figs. 5(a), 5(b), 6(a) and 6(b) show the results from WALKER, in which the neutron under goes a thermal walk. Fig. 7(a) and Fig. 7(b) show the results from RESONANCE, in which nuclear resonances are considered. Fig. 3(a), Fig. 4(a), Fig. 5(a), Fig. 6(a) and Fig. 7(a) show the mean displacement of the neutron as a function of its initial energy. Fig. 3(b), Fig. 4(b), Fig. 5(b), Fig. 6(b) and Fig. 7(b) display the mean time for absorption as a function of the neutron's initial

energy.

The figures from RESONANCE only includes data that uses a constant scattering angle. This is done because each simulation assumes that the scattering angle does not affect the energy lost in a collision. In RESONANCE the neutron energy is what determines if it is absorbed by a resonance or not. So the behavior for the varying scattering angle data and the constant scattering angle data will be the same.

Fig. 2 shows the nuclear resonances taken from the CENDL database. A spike in the cross section indicates a resonance. From Fig. 2, 32 resonances were extracted.

Fig. 3(a) shows the mean displacement until absorption follows a fit given by $R = log(E_i)$. Whether or not this trend is the same in all materials is something that could be studied in the future. Fig. 3 (b) shows that the time for absorption for neutrons with energies above 1keV, is approximately 0.5 ms. For energies lower than 1keV there is a sharp drop in the total time until absorption.

When a varying scattering angle is included into the simulation the distance traveled by neutrons is no longer given by a single value for a particular initial energy, rather by a range of values. By comparing Fig. 3(a) and Fig. 4 (a), we see that some neutrons travel up to 40 cm farther in AVARIETY than they would with a constant scattering angle in ORGIN. This is important because in reality neutrons do not always scatter at the same angle. This variance in displacements makes determining the exact distance a real neutron will travel in a material very difficult.

Comparing the time for absorption in ORGIN, Fig. 3 (b), and AVARIETY, Fig. 4 (b), we see that the time for absorption has no dependence on the scattering angle. This is a direct consequence of the assumption that the scattering angle does not affect the energy lost by the neutron in a collision. Since the neutron's energy is not affected by the scattering angle, both the velocity and the mean free path are also not effected. Since these quantities are constant, we see from Eq. (5) that varying the scattering angle should also not affect the time for absorption.

If this simulation method were to be applied to a substance with a smaller atomic mass, the energy loss would have a greater dependence on the scattering angle. This is because the $m^2_{substance}$ and the $2m_n m_{substance}$ terms from Eq. (2) would be comparable as $m_{substance}$ gets smaller. For example, if this method was used with helium, which has an atomic mass of 2 amu, then the fractional energy loss would vary 7% when the scattering angle is varied 10 degrees. In future studies, the energy lost in a collision could be linked to the scattering angle given by Eq. (2). In fact, if this simulation method was used for less massive nuclei, the energy lost in a collision must be coupled to the scattering angle for accurate results.

Comparing a simulation in which neutrons are immediately absorbed after becoming thermal and one in which thermal neutrons undergo a thermal walk before absorption allows the determination of the effects of the thermal walk on the total distance and time it takes for a neutron to become absorbed. Comparing Fig. 3 and Fig. 4 with Fig. 5 and Fig. 6, we see the same trend is followed for the distance and time until absorption when the thermal walk is and is not included.

To isolate the displacement during the thermal walk, Fig. 3 (a) and Fig. 5 (a) must be compared. In Fig. 5 (a) the difference in displacement from Fig. 3 (a) is purely from the thermal walk and thus

allows us to determine the displacement added from the thermal walk. Comparing these figures we see that there is only a small difference in the total displacement until absorption when the neutron undergoes a thermal walk and so we can conclude that the displacement added while the neutron is thermal is very small. In fact our simulation found on average the thermal walk displacement was 3.43 cm. This value was found by tracking the thermal walk for 1000 neutrons and taking the average.

When comparing Fig. 3 (b) with Fig. 5 (b) and Fig. 4 (b) with Fig. 6 (b), it is clear that the thermal walk has a significant effect on the total time for absorption. In fact for high-energy neutrons there is roughly a 20% increase in the total time for absorption from the simulations where no thermal walk occurred. It is also clear by comparing Fig. 3 (b) with Fig. 5 (b) and Fig. 4 (b) with Fig. 6 (b), that despite a varying angle high energy neutrons take roughly the same time for absorption and also that as the initial energy is decreased the time for absorption is also decreased. Although a precise time cannot be determined for when a neutron will be absorbed, a range can be determined from Fig. 5 (b) and Fig. 6 (b). For neutrons above 1 eV the time for absorption is in the range of 0.5 ms - 0.7 ms and for neutrons below this energy it takes roughly 0.1 ms - 0.5 ms. These values are simply read off of Fig. 5 (b) and Fig. 6 (b).

When nuclear resonances are considered, many high-energy neutrons are captured before becoming thermal. This is clear from Fig. 7 (a) where high energy neutrons only travel a short distance because they have been absorbed. This is a consequence of the width of the resonances, which was assumed to be 0.02% of the energy of the resonance energy. This is a rough approximation that won't give equal resonance widths and must be improved in future studies. Looking at Fig. 2 it is clear the width of each resonance is not the same but this approximation gives us an idea of the effect of resonaceses on the outcome of our simulation

Fig. 7 (a) shows that the neutrons that are absorbed by resonances do not travel as far as those that are absorbed at thermal energies, as is expected. Fig. 7 (b) shows that the time for absorption follows the same trend as the time for absorption with a constant scattering angle and with a varying scattering angle. Neutrons absorbed by a nuclear resonance are absorbed extremely fast, as the line at the bottom right of Fig. 7 (b) shows. These lines at the bottom right appear to be at zero absorption time but this is just a consequence of the scale of the axis.

There are still many ways to improve the simulation method presented. The first improvement would be to have the neutron travel roughly one mean free path during each step rather than exactly one mean free path. The distance neutrons travel in-between collisions is truly given by a distribution of values whose average is one mean free path. This would reflect what occurs in reality better and would result in a larger spread in the total distance and time for absorption.

One could then investigate how changes in the scattering angle change the energy lost in a collision. If the neutron hits the target nuclei directly it will lose more of its energy than if it just graced the side of the nuclei. For this simulation the 2% energy loss was sufficient because ^{136}Xe is a very large nucleus and the scattering angle does not vary more than 10 degrees until the neutron is thermal.

Another improvement to the method would be to consider varying the width of nuclear resonances more accurately. Our assumption that the resonance width is some fraction of the energy of the

resonance is very crude but gives an idea of the effects of resonances. With these further improvements an even more accurate determination of the mean displacement and time for neutron absorption in ^{136}Xe could be made.

4 Conclusion

We have developed simulations that have allowed us to make a rough estimate of the distance and time it takes a neutron of a given initial energy to become absorbed in ^{136}Xe. With background data from the nEXO detector, along with the estimates from our simulation, we can now estimate if neutrons entering the detector will be absorbed within the detector or if it will just pass through. If the neutron will be absorbed within the ^{136}Xe detector, we can determine approximately when the neutron will be absorbed, and therefore can distinguish if an observed decay was truly the $0\nu\beta\beta$ decay or the β decay caused by the neutron absorption.

5 References

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6 Figures

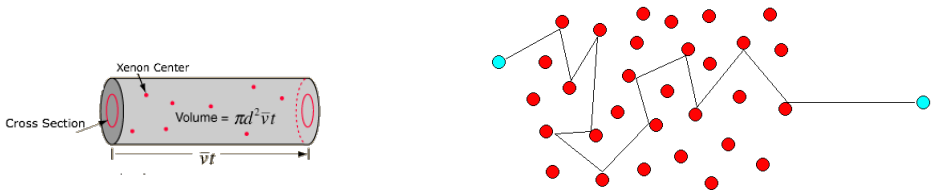

Figure 1: Cylinder of mean free path (left) and visualization of neutron (blue) traveling through ^{136}Xe (in red).