This Is Just the Beginning:
The Hunt for Astrophysical Neutrinos

Dissertation

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By
Weishi Li, B.S.
Graduate Program in Physics

The Ohio State University
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Dissertation Committee:
Professor John F. Beacom, Advisor
Professor Amy L. Connolly
Professor Ciriyam Jayaprakash
Professor Annika H. G. Peter
Abstract

Astrophysical neutrinos are precious messengers of our Universe. They reveal information about the core of the Sun, the interiors of exploding stars, the sites of cosmic-ray acceleration, and fundamental properties of neutrinos. Yet, the study of astrophysical neutrinos has been a difficult quest. Because neutrinos interact only weakly with matter, we need kilo-ton-scale or even larger detectors to detect reasonable numbers of signal events. Modest numbers of signal events are overwhelmed by large numbers of background events, i.e., events that look like neutrinos but they are caused by other processes. On top of that, we are limited in what neutrino properties we can extract from detected events, and with what precision.

In this dissertation, I discuss a series of papers aimed at improving our measurements of astrophysical neutrinos. Solar neutrinos, with energies around 10 MeV, have been detected in Super-Kamiokande for 20 years, yet some key measurement results are still inconclusive. One limiting factor is the spallation background induced by cosmic-ray muons. To better reject this background, I first calculate the spallation yields in Super-Kamiokande. I then study the production mechanisms of spallation backgrounds in detail and conclude that they depend on muon-induced electromagnetic and hadronic showers, rather than by muons themselves. Next, I explore how to reconstruct showers in Super-Kamiokande with high fidelity and propose a new spallation cut utilizing better-reconstructed shower profiles. On the TeV – PeV astrophysical neutrino front, one experimental limitation with current detection techniques is that they cannot distinguish between two neutrino types, or flavors, $\nu_e$ and $\nu_\tau$. To solve this problem, I propose two new shower-related experimental observables, muon echoes and neutron echoes, that are stronger in $\nu_\tau$-initiated events.

The methods presented in this dissertation have been adopted by neutrino experimental collaborations, with results yet to come out. This is just the beginning.
To Lexie, who lives at the tip of my heart
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VITA

2011 ................................. B.S. Physics, The Ohio State University

2011 – 2016 ........................ Graduate Associate, Department of Physics, The Ohio State University

2016 – 2017 ........................ Presidential Fellow, The Ohio State University

Publications

*The Similarity Renormalization Group with Novel Generators,*
W. Li, E. R. Anderson, R. J. Furnstahl,

*First Calculation of Cosmic-Ray Muon Spallation Backgrounds for MeV Astrophysical Neutrino Signals in Super-Kamiokande,*
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*Spallation Backgrounds in Super-Kamiokande Are Made in Muon-Induced Showers,*
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*Tagging Spallation Backgrounds with Showers in Water-Cherenkov Detectors,*
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Chapter 1

INTRODUCTION

Astrophysical neutrinos are precious messengers of our Universe. They have provided us an immense amount of knowledge despite our incomplete understanding of all basic properties of neutrinos and of the fluxes of astrophysical neutrinos. Solar neutrinos provided not only the definitive proof that nuclear fusion powers the Sun, but also evidence for neutrino mixing. Supernova neutrinos from SN 1987A confirmed our theoretical framework of supernova explosions, informing our theories of stellar evolution, and also enabled us to constrain physics beyond the Standard Model. High-energy (TeV – PeV) astrophysical neutrinos are challenging our understanding of the high-energy accelerators of the Universe.

We will learn a lot more from astrophysical neutrinos. We may finally have the experimental sensitivity necessary to measure solar neutrinos from the CNO cycle in Borexino, realizing John Bahcall’s decades-old dream of using neutrinos to precisely probe the Sun, and informing us about how more-massive stars work. We also begin to measure $^8$B solar neutrinos with high precision, complementing next-generation terrestrial neutrino experiments. We are designing the next-generation neutrino experiments suitable for the next Galactic supernova, which will likely lead to thousands of detected events, and to new insights, expected and unexpected, into supernova physics and neutrino physics. Lastly, we are making rapid progress on multi-messenger astronomy and are hopefully on our way to solve the century old mystery of where ultra-high-energy cosmic rays — the most energetic particles in the Universe — are made.

There are also astrophysical neutrino fluxes that have not been detected yet (see Fig. 1.1). These are the least and most energetic astrophysical neutrinos that we believe exist. They are even harder to detect than MeV and PeV neutrinos. At the meV scale, relic neutrinos, survivors of the early Universe, induce feeble recoils in detectors. Above the PeV scale, the expected neutrino flux is so low that we nominally need enormous detectors, with volumes of $10^6$ km$^3$, and long exposures. Despite the challenges, there are on-going experimental efforts to detect neutrinos in both of these extreme energy regimes. While these neutrinos are not the subject of this dissertation, it is only to be expected
that, when they are finally detected, they will open up new fields of study.

The work presented in this dissertation focuses on improving the measurements of solar neutrinos and high-energy astrophysical neutrinos, the two steady-state fluxes of astrophysical neutrinos that we have detected so far. These two fields are in rather different stages of maturity. Solar neutrino studies have been going on for decades and we have a good theoretical understanding of both the solar physics and the neutrino physics involved. Naively, it would seem that the only work left to do is to continue taking data and to marginally improve the measurement precision. (From the interesting abstract of Ref. [30], “... the Organizers entrusted me with a discussion of the provocative question ‘whether solar neutrino physics is over’ ”.) By comparison, the field of high-energy neutrinos is a new one, with first detection in 2012. At this early stage, we do not yet know some of their basic properties, e.g., what astrophysical objects produce them, the precise shape of their energy spectrum, etc. To me, both fields are rich with open questions and physics opportunities; this dissertation serves as an example.

This rest of the chapter is organized as follows. In Sec. 1.1, I present a theoretical overview of solar neutrinos, highlighting open questions in the solar sector and experimental obstacles, motivating my work in Chapters 2, 3, and 4. In Sec. 1.2, I discuss high-energy astrophysical neutrinos, focusing on detection techniques and search strategies, motivating my work in Chapter 5. In Sec. 1.3, I give a brief introduction and summary of my work in this dissertation.
Figure 1.2: Parameter space fitted by solar data (colored contours for GS98 model and black dashed lines for AGSS09 model) and by KamLAND data (solid green lines). Figure taken from Ref. [6].

1.1 Solar neutrinos

Solar neutrinos are made by fusion reactions in the Sun. Their energies are in the range 0 – 20 MeV. They are exclusively produced as $\nu_e$, but, due to neutrino oscillations, they are detected at Earth as either $\nu_e$ or $\nu_\mu/\nu_\tau$. They are excellent probes of the solar core and of the neutrino mixing parameters $\sin^2 \theta_{12}$, $\Delta m^2_{21}$.

1.1.1 Open questions

Despite decades of heroic effort and two Nobel Prizes [31, 32] awarded to solar neutrino physics, we are still in a rather unsatisfying position in solar neutrino physics. We are stuck, experimentally, and hence theoretically. Here is a list of measurements that need to be improved:

- Up-turn region in the spectrum
- Day-night effect

Both phenomena stem from neutrino mixing in matter. (Detailed discussion on oscillations is in Sec. 1.1.3.) The problems can be summarized in Fig. 1.2. Solar neutrinos — from SNO, in particular — give the strongest constraint on $\sin^2 \theta_{12}$, whereas reactor neutrinos — from KamLAND — give the strongest constraint on $\Delta m^2_{21}$. However, the best-fit values of $\Delta m^2_{21}$ found by the solar data and KamLAND disagree at the $\sim 2\sigma$ level. There are two measurements driving this disagreement. First, none of
the solar experiments has measured the predicted up-turn trend in the oscillation probability. Second, the day-night effect measured by Super-Kamiokande is stronger than the prediction made using KamLAND best-fit values. Both measurements have large errors, as seen from the parameter contours in Fig. 1.2. The worst aspect of this disagreement is that there is no obvious way to improve solar measurements in the near future.

- CNO neutrino flux

Solar CNO neutrinos (see Sec. 1.1.2) would be the best probes of solar metallicity, were we to detect them. However, there is no guarantee that Borexino can detect CNO neutrinos. Further, detection needs to occur with sufficient precision to distinguish between a low-metallicity Sun and a high-metallicity Sun. Otherwise, we may fail to deliver on the promise of precisely measuring the Sun using neutrinos.

Percent-level measurements of the above would allow us to precisely test the three-flavor neutrino mixing paradigm. We could also test for new physics models, e.g., non-standard neutrino interactions and sterile neutrinos. Both are popular solutions for the solar-KamLAND discrepancy and, if real, could complicate the long-baseline neutrino program.

It is important to keep in mind the difference in the precision to which we know mixing parameters in the neutrino and quark sectors. Neutrino mixing matrix elements are measured only to 10% to a factor-of-2 precision. In comparison, quark mixing matrix elements are known to sub-percent to percent precision. Clearly, neutrino oscillations are far from being precisely measured, and it should be.

1.1.2 Solar neutrino production

In the solar core (R \( \lesssim 0.25 R_\odot \)) [33], nuclear fusion reactions convert protons into helium nuclei, producing gamma rays and electron neutrinos, and releasing energy. The net reaction is [34]

\[
4p \rightarrow ^4\text{He} + 2e^+ + 2\nu_e + 24.7 \text{MeV}.
\]

The positrons annihilate with electrons immediately after being produced, raising the total energy released to 26.7 MeV. Of that, only 0.6 MeV is carried off by neutrinos [34]. The rest goes into gamma rays and the kinetic energy of nuclei.

The gamma rays and neutrinos both have energies of order MeV, but they propagate differently to the solar surface. The gamma rays constantly get absorbed and re-emitted by the solar plasma, with a mean free path of \( \sim 1 \text{ cm} \) [34]. It takes \( \sim 10^4 \) years for the energy of a gamma ray to propagate to the solar surface, while the gamma ray turns into many photons of visible light [34]. On the other hand, the mean free path of a MeV neutrino is
The pp chain of stellar thermonuclear reactions. The produced neutrinos are typed in boldface characters. The traditional names of the neutrino-producing reactions and the corresponding neutrino fluxes are given in parentheses. The underlined labels indicate the three main branches of the pp chain.

The electron neutrinos produced in the process in eqn (10.2) in the core of the Sun can be detected on the Earth. They provide a unique direct probe of the interior of the Sun.

In order to understand the basic principles of energy generation in the core of the Sun, let us consider a generic nuclear reaction \( A + B \rightarrow \text{anything} \) occurring in a stellar gas where there are \( N_A \) and \( N_B \) particles per unit volume of type A and B, respectively. The cross-section \( \sigma \) of the process in eqn (10.4) depends only on the relative velocity \( v \) and one can consider either A or B as a projectile and the other as a target. Let us consider A as the projectile, with velocity \( v_a \), and B as the target. The rate for a reaction particle A is given by the cross-section \( \sigma \) times the number density \( N_B \) of targets. Since the flux of projectiles is \( N_A v \), the rate for each reaction in eqn (10.4) per unit volume is given by:

\[
\text{Rate} = \sigma N_B \frac{N_A v}{v_a}
\]

Figure 1.3: The solar pp chain. Figure taken from Ref. [7].

\(~ 10^{10} \) km [35]. It takes a neutrino \(~ 2 \) s to reach solar surface, and it does not interact. This is one of the reasons why solar neutrinos are so important: they directly carry the information of the innermost region of the Sun, unlike the photons.

The net reaction proceeds via two groups of interactions, the proton-proton (pp) chain and the CNO cycle, which are shown in Figs. 1.3 and 1.4, respectively. The pp chain provides 99% of the energy of the Sun and the CNO cycle provides 1% [34].

One interesting fact is that all the neutrino-producing reactions occur at slightly different locations in the Sun, as shown in Fig. 1.5. The location where a reaction occurs depends on what the most crucial requirement for that reaction is. For example, \(^8\)B reaction has a high temperature dependence \((\propto T^{20})\) [34], so it happens closer to the solar center where the temperature is higher. On the other hand, the hep reaction rate is proportional to \(^3\)He density, and \(^3\)He has its highest concentration at about 0.2 \( R_\odot \), so hep neutrino production
peaks further away from the center [34]. This difference in production site makes it possible to probe local properties of the Sun using neutrinos.

The reaction rate between two species is [34]

\[ R_{12} = \frac{N_1 N_2}{1 + \delta_{12}} \langle \sigma v \rangle_{12}, \]  

(1.2)

where \( N_i \) is the number density for the \( i \)th species and the angle bracket denotes a thermal average. The \( \delta \) function avoids double counting when the two species are the same. To estimate the neutrino flux from various reactions, we need three pieces of information: the thermal distribution of the reactants, the reaction cross sections and the neutrino spectrum from each reaction.

In the solar core, the velocity distributions of protons and other nuclei can be described by the Maxwell-Boltzmann distribution for an ideal gas [36],

\[ \langle \sigma v \rangle = \int_0^\infty f(E) \sigma v \, dE = \int_0^\infty \frac{2}{\sqrt{\pi}} \frac{\sqrt{E}}{(kT)^{3/2}} e^{-E/kT} \sigma(E) \left( \frac{2E}{\mu} \right) \, dE. \]  

(1.3)

Here \( k \) is the Boltzmann constant, \( T \) is the temperature of the system, \( \mu \) is the reduced mass of the two interacting particles, and \( E \) is the kinetic energy in center of mass frame. The ions can be considered as free particles because the typical Coulomb potential (\( \lesssim 0.1 \) keV) is much less than the thermal energy (\( \sim 1 \) keV). The velocity distribution is in the classical regime because the solar center temperature is much higher than its Fermi energy \( \epsilon_F \sim 10^{-4} \) keV.
The second ingredient, the cross section, is extremely difficult to measure or to calculate. In the solar core, the Coulomb barrier for fusion reactions is $\sim 1$ MeV, much higher than the kinetic energy of a nucleus [37]. The only way these reactions can happen is through tunneling, thus the reaction rates are incredibly low. (This is the reason why the Sun can last so long [34].) Experimentally, low reaction rates mean low signal-to-noise ratio and that it takes a long time to get good statistics. The current method is to express the cross section by [38]

$$\sigma(E) = \frac{S(E)}{E} e^{-2\pi \eta(E)}, \quad \eta(E) = Z_1 Z_2 \alpha \sqrt{\mu/2E}. \quad (1.4)$$

Here $\mu$ and $E$ are the same with those in Eq. 1.3, and $\alpha$ is the fine structure constant. The exponential term is the Gamow factor for tunneling, i.e., the probability of the nuclei penetrating the Coulomb barrier. The geometric factor for the reaction is $\propto \pi \lambda^2 \propto 1/E$, where $\lambda$ is the wavelength of the reduced mass [39]. By assuming that we are left with a smooth function of $S(E)$ (astrophysical $S$-factor), we are able to extrapolate the cross section value from tens and hundreds of keV, which is experimentally approachable, down to the keV energy scale [38].

The velocity distribution and cross section combined give us the energy dependence shown in Fig. 1.6. At low energies, the cross section goes to zero because of the tunneling suppression. At high energies, the Maxwell-Boltzmann distribution has an exponential suppression. Consequently, the energy contribution peaks somewhere in between, and it is called the Gamow peak. A typical value for the Gamow peak is between a few to tens of keV [34]. Figure 1.6 also shows that the Gamow peak is in the tail of both statistical and tunneling functions. This explains why the thermal averaged reaction rates are so low.

The last piece we need is the neutrino spectrum from each reaction, which can be calculated using Fermi’s beta decay theory. Below, we study a standard textbook example, $A \rightarrow B + e^- + \bar{\nu}_e$, with $A$ at rest. This suffices because we only focus on the outgoing

Figure 1.5: Solar neutrino flux as a function of distance to the solar core. Figure taken from Ref. [7].
neutrino spectrum, instead of the full reaction differential cross section. Moreover, because the kinetic energy of the nuclei in the Sun is so small, we can treat them as at rest and still get a good understanding of the problem. Because the decay is caused by a weak Hamiltonian, we can treat it as a perturbation to the quasi-stable initial and final states. The reaction rate can be written using Fermi’s Golden Rule as [39]

$$\lambda = \frac{2\pi}{\hbar} |\mathcal{M}_{if}|^2 \frac{dN}{dE_T}. \quad (1.5)$$

The amplitude term $\mathcal{M}$ can be written as $\langle \Psi_f | V_{int} | \Psi_i \rangle$, where $\Psi$ is the wave-function of the system, and $V_{int}$ is the interaction. The final state contains the residual nucleus, the electron and the neutrino $\Psi_f = \Psi_R \Psi_e \Psi_\nu$ [39]. To the lowest order, the electron and neutrino can be treated as free particles, so their wave-functions are plane waves [40]. Now, the reaction region is roughly the size of the nucleus ($\sim 1$ fm), much smaller than the De Broglie wavelength of the electron ($\sim 600$ fm). We can thus treat the wave-function of the electron and neutrino to be constant when calculating the matrix element. The matrix element then only depends on nuclear physics.

The last factor in Eq. 1.5 describes the final state density, i.e., the number of available states for the system for a fixed disintegration energy $E_T$. For any specific reaction, with all reactants at rest, $E_T$ is always fixed. Ignoring the recoil energy of the nucleus, the disintegration energy goes into electron energy $E_e$ and neutrino energy $E_\nu$ with $E_e + E_\nu = E_T$. Using the state density formula for a Fermi gas, we have [39]

$$dN \propto p_e^2 dp_e p_\nu^2 dp_\nu \delta(E_e + E_\nu - E_T). \quad (1.6)$$

Since both the neutrino and the electron are of order MeV, we get [39]

$$dN \propto E_e (E_e^2 - m_e^2)^{1/2} (E_T - E_e)^2 dE_e. \quad (1.7)$$
Here the spectrum is expressed in terms of the electron energy instead of the neutrino energy, because it is more common in the literature and easier to measure.

So far we have ignored the Coulomb interaction between the outgoing electron and the nucleus. As the electron wave-function is much larger than the size of the nucleus, we can treat the Coulomb interaction as a correction to the value of the wave-function at the origin, $\Psi_0(r = 0) \to \Psi_c(Z, E_e, r = 0)$ [40]. This is described by the Fermi function $F(Z, E_e)$ [40].

In the end, the electron (neutrino) spectrum has the form [40]

$$\lambda(E)dN \propto F(Z, E_e)|M_{if}|^2E_e(E_e^2 - m_e^2)^{1/2}(E_T - E_e)^2dE_e.$$  \hfill (1.8)

This is a reasonable approximation for $pp$, $^8B$, $hep$, and CNO neutrino spectra.

Since $^7Be$ and $pep$ neutrinos are produced in reactions with only two final-state particles, they have line spectra. In this case, we can solve for the outgoing neutrino energy by using momentum and energy conservation. $^7Be$ neutrinos have two possible energies, which corresponds to reactions with two excited state daughter Li states [34].

Putting everything together, we get a theoretical estimation of the solar neutrino flux from different reactions [41–44] as shown in Fig. 1.7. The $pp$ neutrinos are the most abundant, and their energy is the lowest. CNO neutrinos have both moderate energies and fluxes. $^8B$ neutrinos have a low flux, and mainly have energy between 4 – 15 MeV. The $hep$ neutrinos have an extremely low flux.

There is a slight difference in the spectrum shape between $pp$ neutrinos and $^8B$ neutrinos. At high energy, the cutoff of the $pp$ neutrino spectrum is a straight line. For $^8B$ and $hep$ neutrinos, the high energy part falls down smoothly. The difference is due to the different
end-point energy compared to the electron mass. This can be understood with Eq. 1.7. High neutrino energy means low electron energy. If the end-point energy is small compared to electron mass (pp), the spectrum goes as $T_e^{-1/2}$. It is a fast rise for electron spectrum, thus a fast fall for neutrino spectrum. If the end-point energy is high compared to the electron mass ($^8$B and hep), the spectrum goes as $T_e^{-2}$. This corresponds to a slower rise (fall) for electron (neutrino) spectrum.

1.1.3 Solar neutrino oscillation

Solar neutrinos undergo neutrino oscillation after they are produced. It can be approximated by a two-level system. The states involved are $\nu_1$, $\nu_2$, $\nu_e$, and $\nu_\mu$. We show below why this is a good approximation. We adopt the mixing parameters from the Particle Data Group [35], $\sin^2 \theta_{12} = 0.307$ and $\Delta m_{21}^2 \equiv m_2^2 - m_1^2 = 7.53 \times 10^{-5}$ eV$^2$. This is called the large mixing angle (LMA) solution [35]. All the results obtained in this section are calculated assuming the standard mixing parameters.

For a two-level system, the Schrödinger equation in the mass eigenbasis is [10]

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \Psi_1(t) \\ \Psi_2(t) \end{pmatrix} = H_{\text{mass}} \begin{pmatrix} \Psi_1(t) \\ \Psi_2(t) \end{pmatrix} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \begin{pmatrix} \Psi_1(t) \\ \Psi_2(t) \end{pmatrix}. \quad (1.9)$$

For relativistic particles in vacuum:

$$E_i = \sqrt{p_i^2 + m_i^2} \simeq E + \frac{m_i^2}{2E} = E + \frac{m_1^2 + m_2^2}{4E} + \frac{m_i^2 - (m_1^2 + m_2^2)/2}{2E} . \quad (1.10)$$

We drop terms proportional to the identity matrix to make the Hamiltonian traceless. These terms do not contribute to flavor oscillation, because they are proportional to the identity matrix in any basis under unitary transformations. Identity terms in the flavor basis do not mix flavor states. Analogously, neutrino flavor oscillation derives from a phase difference between mass eigenstates, which can develop during propagation. The identity matrix only contributes to the overall phase, so it does not affect flavor oscillation. As a result, the mass basis Hamiltonian can be written as [10]

$$H_{\text{mass}} = \frac{\Delta m^2}{4E} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} , \quad \Delta m^2 = m_2^2 - m_1^2 > 0 . \quad (1.11)$$

In the flavor eigenbasis, the Schrödinger equation has the form [10]

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \Psi_e(t) \\ \Psi_\mu(t) \end{pmatrix} = H_{\text{flavor}} \begin{pmatrix} \Psi_e(t) \\ \Psi_\mu(t) \end{pmatrix} . \quad (1.12)$$
with
\[ H_{\text{flavor}} = \frac{\Delta m^2}{4E} \begin{pmatrix} -\cos 2\theta_v & \sin 2\theta_v \\ \sin 2\theta_v & \cos 2\theta_v \end{pmatrix}. \] (1.13)

Here \( \theta_v \) is the mixing angle in vacuum, \( \theta_v = \theta_{12} \), to distinguish it later with the mixing angle in matter. If a \( \nu_e \) is produced initially, the survival probability of the neutrino is \[ P(\nu_e \rightarrow \nu_e) = |\Psi_e(t)|^2 = 1 - \sin^2 2\theta_v \sin^2 (\pi t/L_{\text{osc}}), \] (1.14)
with oscillation length \( L_{\text{osc}} = 4\pi E\hbar/\Delta m^2 \). Notice that the oscillation amplitude depends on the vacuum mixing angle \( \theta_v \). If the mixing angle was small, we would not get significant vacuum oscillation. For a typical \( ^{8}\text{B} \) neutrino, \( E \simeq 10 \text{ MeV} \), with the LMA parameters, \( L_{\text{osc}} = 3.3 \times 10^5 \text{ m} \). The \( ^{8}\text{B} \) neutrino production site spans \( \sim 0.05 \text{ R}_\odot = 3.5 \times 10^7 \text{ m} \), much larger than the oscillation length. When we calculate the survival probability, we need to integrate over the production location, i.e., averaging over many oscillation periods. As a result, the probability reduces to \( P(\nu_e \rightarrow \nu_e) = 1 - \frac{1}{2} \sin^2 2\theta_v \). This tells us that the neutrino survival probability is independent of neutrino energy. However, this is not consistent with observations of solar neutrinos.

To see how neutrino energy dependence comes into play, we need to understand the Mikheyev-Smirnov-Wolfenstein (MSW) effect [45]. During their propagation in matter, neutrinos can forward scatter on electrons through charged-current (CC) neutrino interactions, mediated by the \( W^- \) boson, and through neutral-current (NC) interactions, mediated by the \( Z^0 \) boson [46]. The NC interactions are flavor-blind, so do not affect neutrino flavor oscillation. However, the CC neutrino scattering on electrons is unique to \( \nu_e \), because there are no muons or taus in the Sun. This adds an extra potential term \( V = \sqrt{2} G_F N_e \) to the Hamiltonian, where \( G_F \) is the Fermi coupling constant and \( N_e \) the electron number density [47]:
\[ H_{\text{matter potential}} = \begin{pmatrix} V & 0 \\ 0 & 0 \end{pmatrix}. \] (1.15)

Together with the energy term, the total Hamiltonian in the flavor basis is [10]
\[ H_{\text{flavor}} = \frac{\Delta m^2}{4E} \begin{pmatrix} -\cos 2\theta_v + \zeta(t) & \sin 2\theta_v \\ \sin 2\theta_v & \cos 2\theta_v - \zeta(t) \end{pmatrix}, \] (1.16)
with
\[ \zeta(t) = \frac{2\sqrt{2} G_F N_e(t)}{\Delta m^2/E} \] (1.17)
and \( \theta_v \) is the mixing angle in vacuum. If we diagonalize the Hamiltonian, the eigenvectors would be the equivalent mass eigenstates \( \nu_1(t) \), \( \nu_2(t) \) in matter. Figure 1.8 shows \( \nu_1(t) \) and \( \nu_2(t) \) as a function of \( N_e \). The new mixing matrix will give the mixing angle \( \theta(t) \) in matter.

Starting from the right side of Fig. 1.8, the local electron density is high, \( \zeta(t) \gg 1 \).
The flavor Hamiltonian is almost purely diagonal and the separation between two mass eigenstates is large. The mixing angle is close to $\pi/2$, which means that a $\nu_e$ is almost a pure $\nu_2$. As the electron density decreases, $\zeta(t)$ decreases. The two mass eigenstates are closest to each other when

$$\zeta(t) = \cos 2\theta \iff N_{e,R} = \frac{\Delta m^2 \cos 2\theta}{2\sqrt{2}G_F E}.$$  \hspace{1cm} (1.18)

Here, the Hamiltonian is purely off-diagonal, and the mixing angle is $\pi/4$. It means that the two mass eigenstates are maximally mixed. This is called the MSW resonance [10]. The corresponding electron density is called the MSW resonance density. As electron density gets smaller, $\zeta(t)$ becomes much less than $\cos 2\theta$. The flavor Hamiltonian is similar to the vacuum case. The mixing angle is equal to the vacuum mixing angle $\theta_v$.

An electron neutrino is produced as a pure $\nu_2$ if the local density is much larger than the resonance density. As the electron density decreases to the resonance density, there are two possible cases. If the electron density varies slowly and the gap is large, the neutrino will stay on $\nu_2$ as it passes through the resonance. This is called the adiabatic case [45]. Notice for adiabatic case, even though there is no mass eigenstate change, there is flavor change caused by change in local mixing angles [45]. The flavor change mainly happens near

Figure 1.8: The mass eigenstates in matter. Figure taken from Ref. [10]
resonance, as the dotted lines show in Fig. 1.8. On the other hand, if the electron density varies fast and the gap is small, there is a probability $P_{\text{hop}}$ (nowadays more commonly called the crossing probability, $P_c$) that the neutrino will jump from $\nu_2$ to $\nu_1$ near the resonance. This is the non-adiabatic case. We define an adiabatic parameter \[ \lambda = \frac{|\Delta E|}{2 \sin^2 \theta / \sin \theta / \sin \theta / \sin \theta} \] (1.19)

If $\lambda \gg 1$ near resonance, the process is adiabatic, $P_{\text{hop}} = 0$. With an exponential electron density profile [35], and the LMA solution, we find that solar neutrinos propagate through the Sun adiabatically [10].

In the end, we can express the survival probability using the Parke formula [48]

$$P(\nu_e \to \nu_e) = \frac{1}{2} \left[ 1 + (1 - 2P_{\text{hop}}) \cos(2\theta_i) \cos(2\theta_v) \right], \quad (1.20)$$

where $\theta_i$ is the local mixing angle where the neutrino is produced. All the dependence on the propagation length $L$ is lost by averaging over phases. The reason is that the typical oscillation length in matter is much smaller than the extent of the production site [46]. The importance of Eq. 1.20 is that it introduces an energy dependence in the oscillation probability. Even if the mixing angle was very small, as it was speculated, there could still be significant oscillation effect. Both $\cos(2\theta_i)$ and $P_{\text{hop}}$ depend on energy. As the hopping probability is negligible for the Sun, it is $\cos(2\theta_i)$ that is responsible for the energy dependence. We can easily check the limiting cases for Eq. 1.20. If it is an adiabatic process, $P_{\text{hop}} = 0$. An electron neutrino is produced at high density, $\theta_i \to \pi/2$, so it will be in the heavier mass eigenstate $\nu_2$. Throughout the propagation, it stays on $\nu_2$. When it reaches the Earth, the probability that a $\nu_2$ will be a $\nu_e$ is $\sin^2 \theta_v$, which is consistent with the Eq. 1.20. If the electron neutrino is produced at low density, $\theta_i$ will be close to $\theta_v$, and it reduces to the vacuum mixing case.

Here is a potentially confusing point. We say that neutrinos have very small cross sections with matter, so they hardly interact. What is the difference between they do not interact, and that they pass through matter changing flavor due to an extra potential? The answer lies in the difference between single hard scattering and coherent forward scattering. When we consider a single neutrino scatter on an electron, the cross section goes as $G_F^2$, and this is negligible. For the matter potential, we consider that a neutrino accumulates a phase factor, but does not lose any energy in each individual scattering. When we add up all the phases, we get an enhancement in the forward direction [49]. The potential term goes as $G_F^2$ [46].

Figure 1.9 shows the survival probability of a 10 MeV electron neutrino, produced at 0.04 $R_\odot$. Both these numbers are chosen because they are typical for $^8$B neutrinos. The line is calculated using an exponential electron density profile for the Sun, integrating the
Figure 1.9: The $\nu_e$ survival probability as a function of detection location. The $\nu_e$ is produced at 0.04 $R_\odot$, with energy 10 MeV (typical for a $^8$B neutrino). The probability is averaged over phases.

Schrödinger equation numerically to get the probability as a function of time. The problem is that the oscillation length in matter is extremely small compared to the solar radius, so the exact result looks like a band in the plot. Instead, I averaged the probability over many oscillations at every point to get a smoother curve. As one can see, the averaged probability decreases from one to its final value before 0.5 $R_\odot$. This is consistent with our previous discussion about flavor oscillation. For a $^8$B neutrino, the electron density at the production site is higher than the resonance density [34]. As it passes through the resonance ($\sim 0.3 R_\odot$) adiabatically, the flavor mixing happens and the survival probability decreases to its final value.

Figure 1.10 shows the electron neutrino survival probability as a function of the neutrino energy. Similar to Fig. 1.9, the numerical line is calculated by sending electron neutrinos with various energies from 0.04 $R_\odot$ to the solar surface, integrating the Schrödinger equation and getting the final survival probability several $R_\odot$ away. The analytic line is calculated by using Eq. 1.20 with $P_{\text{hop}} = 0$. The discrepancy at very low energies is due to numerical problems. At lower energies, the oscillation length is very small. It needs fine time steps to reach small errors. The numerical errors for small energies are $\sim 2\%$.

As we can see, there are three regions in the figure: a low energy region where the survival probability is roughly flat with $P \sim 0.56$, a high energy region where P is flat with $P \sim 0.3$, and a transition region in between. This transition region is often called the up-turn region. The reason for this trend of $P_{ee}$ is the following. $\zeta(t)$ is a function of $N_e/(\Delta m^2/E)$. A higher neutrino energy is equivalent to a higher initial local electron...
density, which corresponds to the lower flat region in Fig. 1.10. When the neutrino energy is low, it is equivalent to a low initial electron density, which is similar to vacuum oscillation case. The transition region in the middle is where the neutrino energy is $1 - 4$ MeV.

If we consider three-neutrino flavor oscillation in matter, there can be two resonances corresponding to two different electron number densities [46]. The second resonance density is $\sim 10^3 / \text{cm}^3 N_A$ [35], much larger than the electron density in the solar core. As a result, the oscillation due to $|\nu_3\rangle$ is similar to the vacuum oscillation case. The large mass difference ($\Delta m_{31}^2$) and small mixing angle ($\theta_{13}$) [35] make the vacuum oscillation due to the third state negligible.

So far we have only considered the matter effect in the Sun. At night, as solar neutrinos reach a detector, they pass through the Earth as well. The muon neutrinos can oscillate back to electron neutrinos, a phenomenon called regeneration [47]. This causes an asymmetry between day and night neutrino survival probability, which is called the day-night effect [47]. As we will see below, even though the day-night effect is only several percent, it provides an extra method to test the neutrino oscillation model. The day-night effect has not been confirmed by any experiments.

A full numerical calculation for the day-night effect is beyond the scope of this thesis. Here we will only discuss the problem under several assumptions. Unlike the Sun, where the electron density varies dramatically, the electron density of the Earth does not change too much [47]. We can get a good understanding of the problem by adopting a constant electron density profile. Another assumption is that by the time solar neutrinos reach Earth, the
different mass wave packets are well-separated and propagate incoherently [47, 50]. The Hamiltonian in mass eigenbasis with a constant matter potential is

$$H_{\text{mass}} = \frac{\Delta m^2}{4E} \begin{pmatrix} -1 + \zeta_E \cos 2\theta_v & \zeta_E \sin 2\theta_v \\ \zeta_E \sin 2\theta_v & 1 - \zeta_E \cos 2\theta_v \end{pmatrix}. \quad (1.21)$$

Here $\zeta_E$ is the average $\zeta(t)$ (see Eq. 1.17) for Earth, which is a constant. We can solve the Schrödinger equation for the mass eigenstate $\nu_2$ just like the vacuum mixing case. In the end, the day-night difference can be written as [47]

$$P_{n-d} \simeq -\frac{1}{2} \cos 2\theta_i \zeta_E \sin^2 2\theta_v. \quad (1.22)$$

For a 10 MeV neutrino, $\theta_i \sim \pi/2$. Taking the electron density in Earth to be 2.8 $N_A/cm^3$ [51], we get $P_{n-d} \sim 2.4\%$. Smaller neutrino energies have a smaller day-night effect. Day-night effect provides a strong constraint on the mixing parameter $\Delta m_{21}^2$.

### 1.1.4 Detecting MeV neutrinos

Neutrino detection is difficult due to extremely small cross sections. To get statistically significant signals, we need large detectors and careful background reduction. Starting from the 1950s, we have had Homestake, Kamiokande, GALLEX/GNO, SAGE, Sudbury Neutrino Observatory (SNO), Super-Kamiokande (Super-K), and Borexino solar neutrino experiments.

Many experimental results can be summarized in Fig. 1.11. The plot shows the solar
electron neutrino survival probability as a function of energy, just like Fig. 1.10. The MSW-LMA prediction is from the SSM neutrino fluxes and three flavor neutrino oscillation model with the standard mixing parameters. The MSW-LMA line is very similar to the one in Fig. 1.10, because as we have explained before, three flavor mixing gives similar result to two flavor mixing.

One can see that solar neutrino measurements are in good agreement with our theoretical prediction. However, the experimental precision is far below the theoretical precision. In the most interesting region, the up-turn region, the survival probability is only loosely bound from low energies by the pep measurement with a significant error bar, and bound from high energies with two energy-integrated measurements on $^8$B neutrinos. As a consequence, the error on $\Delta m^2_{12}$ is $\sim 20\%$ if we use only solar neutrino data [6].

The main reasons preventing a more precise measurement are neutrino interaction kinematics and experimental backgrounds. In the following discussion, we focus on the two biggest running experiments, Super-K and Borexino. We first briefly describe how they work, then discuss the issues with kinematics and backgrounds.

Borexino is a liquid-scintillation experiment [11]. It detects neutrinos through neutrino electron scattering:

$$\nu + e \rightarrow \nu + e.$$  \hspace{1cm} (1.23)

The recoil electron gains energy comparable to the neutrino energy and emits scintillation light, which is then detected by photomultipliers (PMTs) surrounding the detector. Scintillator detectors (Borexino and KamLAND) typically have large light yield ($\sim 200$ p.e. per MeV), hence low energy thresholds. This makes Borexino ideal for detecting $^7$Be, pep, and even CNO neutrino. The two experimental points in the transition region in Fig. 1.11 are from Borexino. This is the lower end of the transition region. Note that these two points do not have horizontal error bars because these two reactions produce neutrino line spectra. Borexino is currently trying to perform the first detection of CNO neutrinos.

Super-K is a water-Cherenkov experiment [14] (Fig. 1.12). It has a fiducial (useful) volume of 22.5 kton. It also detects neutrinos through neutrino electron scattering. The recoil electron is detected by its Cherenkov light. Cherenkov light typically has a lower photon count ($\sim 7$ p.e. per MeV), so the energy threshold is higher. On the other hand, water is much cheaper than scintillator, so water detectors can be larger. This makes Super-K ideal to measure $^8$B neutrinos. For $^8$B neutrino, the survival probability should start rising on the left (up-turn). However, as shown in Fig. 1.11, the best fit results from both SNO and SUper-K are rather flat (if not decreasing).

Another key difference between water detectors and scintillator detectors is on directionality. Because Cherenkov light emission is forward whereas scintillation light is isotropic, Super-K can measure the direction of the recoil electrons and Borexino cannot. This gives Super-K an extra handle on background rejection. Next, we use Super-K as an example to
super-K cannot measure neutrino energy event by event. Because the neutrino and electron scattering is a two-body problem, two independent pieces of information are needed to reconstruct the neutrino energy. Super-K can measure the recoil electron energy. MeV electrons lose energy by ionization, and the Cherenkov light intensity is proportional to ionization energy loss. The other required quantity is the recoil electron direction relative to the incoming neutrino direction. (The outgoing neutrino cannot be detected.) This requires higher angular resolution than what Super-K can achieve. Thus, reconstructing the neutrino energy spectrum from only the recoil electron energy spectrum is very important.

Neutrino electron scattering is sensitive to all flavor neutrinos, with \( \sigma(\nu_e)/\sigma(\nu_{\mu,\tau}) \sim 6 \) [34]. The cross section is shown in Fig. 1.13 left panel. The cross section goes linearly with neutrino energy, with value \( \sim 10^{-43} \text{cm}^{-2} \). We can estimate the cross section using the following dimensionality arguments. Since this is a weak interaction, we expect \( \sigma \propto G_F^2 \).

The cross section has dimension \( [E^{-2}] \) and \( G_F \) also has dimension \( [E^{-2}] \). Hence, we need \( \sigma \propto G_F^2 \cdot E^2 \). The only \( [E^2] \) quantity that makes sense here is the invariant mass \( s \). As a result, we have \( \sigma \propto G_F^2 s \). When \( E_\nu > m_e \), \( s \simeq 2E_\nu m_e \). In the end, we get

\[
\sigma \propto G_F^2 E_\nu m_e \sim 10^{-43} \left( \frac{E_\nu}{10 \text{ MeV}} \right) \text{cm}^2.
\] (1.24)

The event rate at Super-K is \( \sim 15/\text{day} \) [52], assuming the \(^8\text{B} \) neutrino flux at Earth to
Figure 1.13: Left: the total cross section for neutrino electron scattering as a function of neutrino energy. Right: the differential cross section for neutrino electron scattering for a 10 MeV neutrino.

be $2 \times 10^6 \text{cm}^{-2} \text{s}^{-1}$. It seems unfortunately small compared to the cosmic-ray muon rate (2 Hz) at Super-K [25], which is responsible for their dominant background events, which we will discuss later. The facts that all flavor neutrinos produce the same signals and that the detection reaction is less sensitive to muon and tau neutrinos are why Super-K counted less solar neutrinos than predicted from SSM. As shown in Fig. 1.11, for neutrinos above the Super-K threshold, the survival probability is about 0.3. The other 70% become muon neutrinos. As a result, Super-K only detected $30\% + 70\% \times \frac{1}{6} \sim 40\%$ of the expected events [34].

For a fixed incoming neutrino energy, the recoil electron also has an energy spectrum. The differential cross section is shown in Fig. 1.13 right panel. It is only slightly dependent on the electron recoil energy, because the outgoing electron has an equal probability to be anywhere below the incoming neutrino energy. We can easily see now why the total cross section is a linear function of neutrino energy. The higher the neutrino energy, the larger the phase space for the electron.

Unfortunately, the relatively flat differential cross section makes it hard to reconstruct the neutrino spectrum. Figure 1.14 shows the electron recoil spectrum for $^8\text{B}$ neutrinos on the right. It represents the convolution of the original $^8\text{B}$ neutrino spectrum (left panel) with the differential cross section (Fig. 1.13). The recoil electron spectrum shape is easy to understand. For a fixed electron energy, any neutrinos with energy above that contribute with equal probability (flat differential cross section). As a result, the event rate at any
Figure 1.14: Left panel: $^8$B neutrino spectrum. $^8$B neutrino spectrum taken from Ref. [13].
Right panel: the recoil electron spectrum for $^8$B neutrino.

electron energy measures the neutrino flux above that energy. It is the opposite to the
cumulative distribution function of the neutrino flux. It does not directly reflect the neutrino
spectrum. If we want to look for any distortion in the neutrino spectrum related to neutrino
oscillation, the distortion will be smeared out by the scattering cross section. The fact that
the recoil spectrum is a falling function of energy also means that most of the events happen
with low electron energy. If the detector threshold were 0.5 MeV, the total event rate would
be $\sim 70$ per day. The threshold is about 5 MeV. That corresponds to a total of $\sim 20$ per
day, which is consistent with the previous quoted number.

Other than kinematic smearing, Super-K and Borexino also suffer significantly from
backgrounds. As the only detectable signature from a neutrino interaction is a recoiled
electron, any electrons in the right energy range from other interactions is a background.
Unfortunately, the background rate is much higher than the signal rate. I will categorize
backgrounds into three types: events that are not actually electrons, electron events from
radioactivities, electron events from cosmic-ray muon-induced spallations. After cuts, which
are algorithms to reject background events from the data sample, the dominant backgrounds
are the latter two types.

Figure 1.15 shows the Super-K event rate as a function of the recoil electron direction.
The total event number is the area under the curve. The solar neutrino events are in the
dark shaded region, where they peak away from the Sun at $\cos\theta_{\text{sun}} = 1$. The light shaded
band shows the isotropic background events. The area of the light region is much larger than
that of the dark region, meaning $N_{\text{bck}} \gg N_{\text{sig}}$. In Super-K, the dominant backgrounds are
radioactive decays at lower energies ($\lesssim 5$ MeV). Between $6 - 18$ MeV, the main backgrounds after cuts are cosmic-ray muon-induced spallation [25]. If the spallation background can be greatly reduced, Super-K will have a much better sensitivity to $^8$B neutrinos.

I will now describe spallation backgrounds in detail, because they are the focus of the bulk of my work in this dissertation. Spallation backgrounds, also called cosmogenic backgrounds, are beta decays of unstable nuclei produced by cosmic-ray muons interacting with detector material. For example, in Super-K, a high-energy cosmic-ray muon can break up an oxygen nucleus, and produce a $^{12}$B nucleus. This $^{12}$B then decays, emitting a 10 MeV electron. This electron looks just like a recoil electron from solar neutrino scattering, making it a background event.

This type of backgrounds can only be produced by cosmic-ray muons, and not protons or other particles. Protons or other hadrons have large interaction cross sections with matter, and can be easily stopped (or shielded) by a layer (maybe a few meters) of material. Muons interact with matter too, but they are able to travel longer distances without being destroyed. Most neutrino experiments are underground ($\sim$ km of rock) to reduce the cosmic-ray muon flux in the detector. It decreases roughly exponentially as a function of the detector depth. Of course, we cannot put all neutrino experiments deep enough underground because it gets very expensive. Super-K is 1 km underground, with a muon rate of $\sim 2$ Hz.

These muons can be easily tagged in solar neutrino experiments. The average muon energy in both Super-K and Borexino is on the order of 300 GeV. When a muon enters a detector, it typically has enough energy to go through it, emitting lots of light.

If an unstable isotope is produced when the muon goes through the detector, it will decay roughly after its lifetime. If an electron event occurs close to a previous muon track in location and in time, it is more likely to be a spallation background. The difficulty to
tag spallation backgrounds rises from the fact that several isotopes produced in water or scintillator have very long lifetimes compared to the muon rate. One dominant background in Super-K, $^{16}\text{N}$, has a lifetime of 7 s! It is easy to imagine that if we consider all electron events happening within 7 s of any muon, and the muon rate being 2 Hz, we would classify all events including neutrino signals as spallation backgrounds. So, given that we cannot move an experiment deeper underground once it is built, how to better reject spallation backgrounds? That is the focus of my study.

To conclude the solar neutrino section, solar neutrino studies have made important contributions to our understanding of neutrino oscillation, but it is far from perfect. We are excited to see what progress we can make in the next few years.

### 1.2 High-energy astrophysical neutrinos

July 2012 marks the beginning of a new era for neutrino astronomy: the IceCube Collaboration announced the detection of Bert and Ernie, two PeV neutrinos of astrophysical origin [53]. Since then, we have made tremendous progress on studying TeV – PeV astrophysical neutrinos. Experimentally, IceCube has now detected a flux of high-energy astrophysical neutrinos from a variety of channels. Theoretically, we have learned about the potential sources of these astrophysical neutrinos and their connection to the gamma-ray sky.

In this section, I will describe what we know about these neutrinos. Opposite to solar neutrinos, where we predicted the flux before measuring it, for high-energy astrophysical neutrinos, we first detected them, and we are still trying to figure out how and where they are produced. So, I will start with the detection of high-energy astrophysical neutrinos and then briefly discuss how we are trying to learn about their sources.

#### 1.2.1 Detecting TeV – PeV neutrinos

IceCube is an ice-Cherenkov experiment with a volume of 1 km$^3$ in Antarctica [17] (see Fig. 1.16). The detector comprises 86 strings, each with 60 optical sensors buried underground between 1450 m and 2450 m. Every optical sensor hosts one PMT. IceCube detects charged particles through their Cherenkov light emission, similar to Super-K. Unlike Super-K, the photo coverage of IceCube is sparse, meaning that most photons do not reach the PMTs. As a result, the detection threshold of charged particles in IceCube is $\sim 100 \text{ GeV}$ [54], way above their Cherenkov threshold.

Between TeV and PeV, neutrinos interact with matter mainly through deep inelastic scattering. It can occur via charged-current (CC) interactions,

$$\nu_l + N \rightarrow l + X,$$  \hspace{1cm} (1.25)
where \( N \) is a nucleon in ice. The final-state hadrons \( X \) represent many charged and neutron pions. The total cross section of the CC channel is shown in Fig. 1.17. The figure covers a wide range of neutrino energies. Below 10 TeV, \( \sigma_{\nu N} \propto E_\nu \). Using similar arguments presented in Sec. 1.1.4, we get

\[
\sigma_{\nu N} \sim 10^{-34} \text{cm}^2 \left( \frac{E_\nu}{10 \text{ TeV}} \right),
\]

(1.26)

roughly consistent with Fig. 1.17. Above a few tens of TeV, this linear relation breaks down. The transferred momentum squared \( Q^2 \) starts to approach \( m_W^2 \), so the cross section is modified by a factor of \( (1 + Q^2/m_W^2)^{-2} \) [7].

The outgoing particles carry energies

\[
E_l = (1 - y)E_\nu, \quad E_X = yE_\nu,
\]

(1.27)

respectively, where \( y \) is called inelasticity. The differential cross section \( d\sigma_{\nu N}/dy \) is shown in Fig. 1.18. For neutrinos at all energies, the differential cross sections peak at \( y = 0 \), i.e., it is most likely that the outgoing lepton carries all the neutrino energy. However, the peaks are rather broad. At 1 PeV, the average \( \langle y \rangle \sim 0.3 \), and it increases as the neutrino energy decreases [16].

Anti-neutrinos interact similarly to neutrinos, with the difference being that \( \nu \) couples to \( d \) and \( \bar{u} \) quarks and \( \bar{\nu} \) couples to \( u \) and \( \bar{d} \) quarks. Because these quarks have different momentum distributions in nucleons, the \( \bar{\nu}N \) interaction has a \( \sim 6\% \) lower total cross
section than the $\nu N$ interaction, and a lower $\langle y \rangle$ below 1 PeV [16].

Both $l$ and $X$ leave detectable signatures. $X$ induces hadronic showers; it is a cascade process of pions multiplying in numbers. It also produces abundant electrons and positrons, which emit Cherenkov light. So, there is always a blob of prompt light at the neutrino interaction vertex. An outgoing $e$ makes an electromagnetic (E.M.) shower; it is a cascade process of electrons and positrons multiplying in number. The E.M. shower combines with the hadronic shower from $X$ and makes a cascade event at the interaction vertex (see Fig. 1.19). An outgoing $\mu$ leaves a long, thin track and it generally travels a distance larger than the detector (see Fig. 1.19). The $\tau$ case is the most complicated one. The $\tau$ decays on a distance scale of [35]

$$L = 50 \text{ m} \left( \frac{E}{1 \text{ PeV}} \right). \quad (1.28)$$

If the $\tau$ energy is lower than 1 PeV, the decay vertex is basically indistinguishable from the neutrino interaction vertex. The $\tau$ then decays with many different branches. 17.8% of the time the $\tau$ decays into $e^-\bar{\nu}_e\nu_\tau$ [35], which looks like a cascade event due to the $e$-initiated shower; 17.4% of the time the $\tau$ decays into $\mu^-\bar{\nu}_\mu\nu_\tau$ [35], which leaves a muon track; the rest of the time, decays are into many hadrons [35], and look like a cascade event due to hadronic showers. If the $\tau$ energy is above 1 PeV, then the decay vertex can be distinguished from the neutrino interaction vertex. In this case, we can get all kinds of interesting event topologies [27, 55, 56].
\( q_0(x, Q^2) = [\nu v(x, Q^2) + d v(x, Q^2)]^2 + [u s(x, Q^2) + ds(x, Q^2)]^2 \) 
\( (R^2 u + R^2 d) \) 
\( + [u s(x, Q^2) + ds(x, Q^2)]^2 \) 
\( (L^2 u + L^2 d) \) 
\( + (1/2) [s s(x, Q^2) + b s(x, Q^2)] (L^2 d + R^2 d) \) 
\( + [c s(x, Q^2) + t s(x, Q^2)] (L^2 u + R^2 u) \) 

Figure 1.18: Neutrino-nucleon CC interaction differential cross sections. Figure taken from Ref. [16].

Similarly, neutrinos can also interact via neutral-current (NC) interactions:

\[ \nu_l + N \rightarrow \nu_l + X. \]  

(1.29)

Again, \( X \) indicates final-state hadrons. In this case, we do not see the outgoing neutrino, so we only detect the cascade induced by \( X \) at the interaction vertex.

IceCube does not have complete sensitivity to separate neutrino flavors at the event level. A track event is very likely to have come from a \( \nu_\mu \) interaction, with a small probability of it coming from a \( \nu_\tau \). But a cascade event could be produced by the CC interactions of either \( \nu_e \) or \( \nu_\tau \) (if the energy is below PeV), or it could be a NC interaction. From the prompt light alone, there is no way to break this \( \nu_e-\nu_\tau \) degeneracy. In Chapter 5, we propose a new experimental technique, designed to break this \( \nu_e-\nu_\tau \) degeneracy for cascade events.

How well we can extract information of the incoming neutrino varies for different event topologies. At the relevant energies, muon tracks can travel farther than the size of the detector. This means that we can measure their direction quite well, \( \sim 0.5^\circ \) at 100 TeV [57]. And, we can detect muons coming from \( \nu_\mu \) interacting outside the detector, which gives the muon track channel a larger effective detector volume. But this also means that we do not have a calorimetric energy measurement of the muon, resulting only a \( \sim 30\% \) energy resolution at 100 TeV [54], and an even worse estimation on the energy of the neutrinos. Particles showers, on the other hand, occur over a distance of \( \sim 5 \) m [3], which is effectively point-like in the detector. (The vertical PMT spacing in one string is 17 m [54].) So, cascade events can only be detected if the neutrino interacts inside the detector. Due to the calorimetric energy measurement, we have an energy resolution of 8\% at 100 TeV [54].
Figure 1.19: Cascade (left) and track (right) events in IceCube. Figure taken from Ref. [17].

But we cannot measure the direction of the shower well; the angular resolution is $\sim 10^\circ$ at 100 TeV [19]. An actual cascade event in IceCube looks significantly larger than $\sim 5$ m. This is due to significant light scattering. In fact, around 50% of the light is concentrated on a handful of the PMTs near the shower vertex [58].

IceCube has a few different analysis channels to search for astrophysical neutrinos. A good summary is given in Ref. [18]. The few important variables are event topology (using only track events, shower events, or both), incoming direction (if they consider only events from one hemisphere or both), and energy threshold.

A clear choice for event topology is to use tracks only, both through-going tracks and starting tracks. As noted, tracks have large range, so this channel has a larger effective volume. However, this channel suffers from significant backgrounds for downward-going tracks. Downward-going tracks from neutrino interactions look just like cosmic-ray muons going through the detector, only with a much smaller rate. So, for track analyses, a clean search uses upward through-going and starting tracks. References [59, 60] are such analyses.

Another choice is to use showers only. The showers used must be contained inside the detector. Because there is no cosmic-ray muon background, shower searches can be full-sky. References [61, 62] are such analyses.

However, shower-only searches can be clearly improved by including starting track events. If we require the primary vertex to be inside the detector, track and shower channels have the same effective volume. By including track events, we increase our event sample...
without introducing significant complications. References [17, 19, 20] are such analyses.

Here is an obvious question with an non-obvious answer: if we restrict ourselves to upward events, do through-going plus starting tracks have better sensitivity than showers? One might guess the answer is yes, due to the larger effective volume. However, the shower channel is actually the more sensitive one. In the relevant energy range, the atmospheric electron neutrino flux is $\sim 1/20$ of the atmospheric muon neutrino flux. (The additional shower background from atmospheric muon neutrino NC interactions are suppressed by an order of magnitude due to cross sections and interaction kinematics.) Consequently, the shower channel is much cleaner [63].

The last variable in searches is energy threshold, which obviously affects all of the search channels above. Choosing an energy threshold involves striking a compromise between conserving the signals and cutting down the backgrounds. In order to understand this, let’s take a look at what the signal flux looks like.

### 1.2.2 Astrophysical neutrino flux

In this subsection, I describe briefly the key features of the astrophysical neutrino flux and discuss their implications.

Figure 1.20 shows the fitted spectra of different fluxes of neutrinos from the IceCube Collaboration. The $x$-axis is neutrino energy, from 10 TeV to 10 PeV. At the low-energy end, the IceCube sensitivity extends to $\sim 100$ GeV, eventually cuts off by trigger efficiency [54], i.e., by running out of detected photons. At the high-energy end, the IceCube sensitivity extends to much higher energies, in principle, but cuts off in practice around a few PeV due to finite exposure. The $y$-axis is the neutrino flux $\Phi_\nu$ multiplied by $E_\nu^2$. The diffuse astro-
physical neutrino flux goes $\sim E^{-2}$, so multiplying the flux by $E^{-2}_\nu$ makes the astrophysical neutrino flux looks flat.

The blue line in Fig. 1.20 shows the conventional atmospheric neutrino flux. High-energy cosmic-ray protons and nuclei (with flux proportional to $E^{-2.7}$) interact with the Earth atmosphere, producing pions and kaons that have the same spectral index. These decay and produce neutrinos. Because pions and kaons lose energy before they decay, the neutrino spectrum is softer than that of the mesons, $\sim E^{-3.7}$.

The green line in Fig. 1.20 shows the upper limit on the prompt atmospheric neutrino flux. Prompt neutrinos are made by charmed mesons produced in cosmic-ray proton interactions in the atmosphere. Charmed mesons barely lose energy before they decay to neutrinos (hence the name prompt), because of their extremely short lifetimes. The consequence is that the spectrum of the prompt neutrino flux closely follows that of the cosmic-ray protons, $\sim E^{-2.7}$. The production rate of charmed mesons is much lower than that of pions and kaons, so the prompt flux is significantly lower. This is why we only have a limit on the prompt neutrino flux, not a definitive measurement yet.

Lastly, the orange band in Fig. 1.20 shows the astrophysical neutrino flux. The best-fit spectrum now has a spectral index of $\sim E^{-2.5}$. Different analysis channels give slightly different results for the spectral index. The spectral index of the astrophysical neutrino flux is particularly interesting for a few reasons. First, the naive expectation of an astrophysical flux is a $E^{-2}_\nu$ spectrum. This is simply because we expect the protons in astrophysical accelerators to have a $E^{-2}_p$ spectrum, from their undergoing Fermi acceleration. A measured spectral index that deviates significantly from that, e.g., $E^{-2.9}$, is interesting. Second, in order to figure out the origins of these neutrinos, we need to rely on observations of other cosmic messengers in other energy range, e.g., GeV gamma-ray observation from Fermi. Extrapolation over orders of magnitude energy involved. Spectrum indices of 2 or 2.9 could yield qualitative different conclusions.

Finally, Fig. 1.20 illustrates the problem of choosing an energy threshold for astrophysical neutrino searches. Atmospheric neutrinos are always a background for astrophysical neutrinos. At low energies, their flux is orders of magnitude higher than that of astrophysical neutrinos. There are some other parameters we can use to distinguish them on a statistical basis, i.e., angular distribution, which we will discuss next, but they do not have 100% efficiency. So, due to the overwhelming atmospheric neutrino rate, a low analysis threshold means more astrophysical neutrino signals, but also more atmospheric contamination.

Another important observable of is the incoming direction. Figure 1.21 shows the zenith angle distribution of IceCube events. Zenith angle $\theta$ is usually labeled such that downgoing events, i.e., events from the southern sky, have $\theta \in (0, \pi/2)$ or $\cos \theta \in (0, 1)$. In this figure, the $x$-axis uses $\sin \delta_{rec} = -\cos \theta$, i.e., the southern sky is on the left side.

In the left panel of Fig. 1.21, the dominant component around 1 TeV is conventional
One of the most exciting aspects of high-energy astrophysical neutrinos is their origins. We do not know what class(es) of astrophysical objects produce them. This is made more interesting for figuring out the origins of the astrophysical neutrinos, which we will discuss in the next subsection.

Atmospheric neutrinos, shown in yellow. Its distribution peaks at the horizon (\(\sin \delta = 0\)), where the atmospheric density is lowest and where pions and kaons lose the least energy. There are fewer events coming from the southern sky because atmospheric neutrinos are typically accompanied by muons, which can be vetoed. The red-shaded band shows cosmic-ray muons coming from the southern sky. These are the muons that do not lose much energy when they enter the detector, and subsequently experience a huge energy-loss interaction, which is mis-reconstructed as a neutrino interaction vertex. On top of the red band sits a blue layer of astrophysical neutrinos. To first order, they are isotropic on the sky, i.e., they show a flat distribution in \(\sin \delta\). Not shown in this figure is the prompt neutrino flux. Like for astrophysical neutrinos, it is also isotropic.

In the right panel of Fig. 1.21, the only surviving component above 100 TeV is from astrophysical neutrinos in blue. It still looks rather flat (isotropic), except towards \(\sin \delta = 1\), i.e., up-going neutrinos transversing the whole Earth. There, neutrino attenuation inside the Earth plays an important role. We can estimate the cross section needed for neutrinos to interact once in Earth:

\[
\sigma_{\text{abs}} \times N_N \times 2R \simeq 1 \iff \sigma_{\text{abs}} \simeq 2.4 \times 10^{-34} \text{ cm}^2,
\]

where we take the Earth radius to be \(R = 6371\) km and the average density to be \(5.51\) g/cm\(^3\) [51]. This corresponds to a neutrino energy of 100 TeV [64], consistent with Fig. 1.21. If one is interested in a careful prediction of neutrino flux transversing Earth, it is important to remember that neutrinos underwent NC interactions do not just disappear, they simply lose energy and show up in the lower energy end of the spectrum. The zenith angle distributions can be used to distinguish astrophysical neutrino signals from conven-
Figure 1.22: Sky map of 3 years of IceCube events. Track events are labeled with × and shower events are labeled with +. Figure taken from Ref. [20].

Additional atmospheric neutrino backgrounds at low energies, and they can test neutrino cross section at high energies [65].

If we manage to select a relatively clean sample of astrophysical neutrinos, we can use sky maps to assess more clearly whether they are isotropic. Figure 1.22 is one such example. Unlike the zenith angle distributions, which are useful for extracting signals, sky maps are particularly interesting for figuring out the origins of the astrophysical neutrinos, which we will discuss in the next subsection.

Sky maps are typically drawn in Galactic coordinates. This means that the Galactic plane is the central horizontal line, and the Galactic center is in the center of the figure. There are quite a few interesting things one can do with such sky maps. The most obvious one is to see if the events are isotropic, looking for clusters around one particular source, or dipole asymmetry. This leads us to the following subsection.

1.2.3 Who ordered that?

One of the most exciting aspects of high-energy astrophysical neutrinos is their origins. We do not know what class(es) of astrophysical objects produce them. This is made more interesting by the connection between these neutrinos and cosmic-ray protons and nuclei. We have detected cosmic rays for over a century, yet we still do not know their sources. Up to PeV, we believe cosmic rays are produced by Galactic sources such as supernova remnants, though we do not have solid evidence. At ultra-high energies, $10^{19}$ eV and above, we do not know what could produce cosmic rays.

One challenging aspect of studying the sources of cosmic rays is that cosmic rays deflect
in magnetic fields. The Larmor radius of a relativistic single-charged particle is

$$r_g = 3.3 \text{ m} \left( \frac{E}{\text{GeV}} \right) \left( \frac{T}{B} \right).$$ (1.31)

In our Galaxy, the cosmic-ray energy is moderate (e.g., $E = 1$ PeV), and the magnetic field is $B \sim 6 \mu$G. So, the Larmor radius $r_g \sim 0.18$ pc, much smaller than length scales of a galaxy. Because of the bending of trajectories, to first order, any information on the true injection position of a cosmic-ray proton is erased when it reaches us. Outside our Galaxy, the energy of a cosmic ray can be extremely high (e.g., $E = 10^{19}$ eV), with a typical magnetic field of $B \sim 1$ nG. The Larmor radius $r_g \sim 11$ Mpc, larger than the expected coherence length of intergalactic magnetic fields. In this case, the typical angular deflection can be expressed as [66]:

$$\theta \simeq 0.8^\circ Z \left( \frac{10^{20} \text{ eV}}{E} \right) \left( \frac{r}{10 \text{ Mpc}} \right)^{1/2} \left( \frac{l_c}{1 \text{ Mpc}} \right)^{1/2} \left( \frac{B}{1 \text{ nG}} \right).$$ (1.32)

So, the deflection of a $10^{19}$ eV proton is still quite significant. Because of this, using neutral particles as probes of high-energy sources seems like an appealing idea.

Gamma rays are one such candidate. Since the *Fermi* Large Area Telescope [67] launched, we have gathered extensive information on the GeV gamma-ray sky and identified many gamma-ray sources. TeV gamma-ray observation is more challenging, due to reasons similar to neutrino observation. Typically, astrophysical fluxes decrease as a power law of the energy, often with a spectrum index of 2 – 3, with a cutoff at the highest energies. The higher the energy, the lower the flux, and the larger detector needed. A new generation TeV gamma-ray telescopes have recently come online, and they should be able to survey our TeV gamma ray sky with unprecedented resolution. If we want to use gamma ray to probe even higher energies, we run into two difficulties: first, we have yet to build a PeV
gamma-ray telescope; second, PeV gamma rays have an attenuation length of $\sim 10$ kpc, comparable to the distance between us and the Galactic center. Because of this, neutrinos have a relative advantage to gamma rays as cosmic messengers. (see Fig. 1.23)

Thanks to the ability of neutrinos to point back at their sources, one can look for neutrinos pointing at a class of potential sources. IceCube carried out such analyses for gamma-ray bursts [68–72]. Another type of search, using the diffuse flux, is to look for two or more events coming from the same region, i.e., cluster. There are several analyses carried out this way [57, 73–76]. Or we can correlate the neutrino sky map with other types of sky map, e.g., gamma rays, galaxy distribution, gravitational lensing, etc, and see if there is any correlation between two of such maps. There are also quite a few analyses carried out this way, e.g., Refs. [77–81]. So far, all such searches have given null results.

Five years after the discovery of high-energy astrophysical neutrinos, we have learned much about them, yet there is so much more to learn.

1.3 My work

In this section, I recap the motivations and give an overview of the key ideas for my work in this dissertation.

Chapter 2 is the first paper of a series aiming at improving the rejection of spallation backgrounds in Super-K for solar neutrino detection. In the first paper, we calculate the spallation background yields. Solar neutrino searches suffer significantly from spallation backgrounds between 6 to 18 MeV (Sec. 1.1.4). This (total) background was crudely measured when Super-K first designed their spallation cuts around the year 2000. A theoretical calculation was considered not possible at that time, due to the complicated nuclear physics involved. Since then, our ability to simulate the relevant processes, especially nuclear interactions, has drastically improved. The most commonly used tools are simulation packages like FLUKA and GEANT4. A few years ago, scintillator experiments KamLAND [82] and Borexino [83] carried out detailed studies of spallation background, both by measurements and by simulation. They found good agreement between the theory predictions and the measurements at a factor-of-2 level. This inspired us to calculate the spallation yields in water.

We simulate muons interacting with water using FLUKA [84, 85]. The most important result is the individual isotope yields in water. We then check our results against all measurements that we can find. At that time, the only studies in water were on $^{16}$N yield, to which we compare our results.

One of our main goals is to encourage Super-K to carry out a detailed measurement of spallation yields. Super-K did perform such a measurement, in Ref. [86].

Chapter 3 is the second paper in the series. Here, we study in detail the production
mechanisms of spallation backgrounds and conclude that they are made in cosmic-ray muon-induced (mostly hadronic) showers.

The conventional picture of muons producing isotopes is that a high-energy muon interacts with an oxygen nucleus directly, breaks it up, and produces a new unstable isotope. This was questioned when one Super-K analysis measured the muon Cherenkov light profiles, often observed wide peaks in these profiles, and subsequently found correlations between these peaks and spallation backgrounds [26], which could not be understood. We set out to explain the origin of these light-profile peaks and their correlation with spallation backgrounds.

We discover that although the conventional spallation mechanism does take place, it only contributes a few percent of the isotopes. More often, a cosmic-ray muon interacts with water, emitting a high-energy (∼10 GeV) secondary particle, such as an electron or a pion. This secondary particle then induces an electromagnetic or a hadronic shower, which produces pions and neutrons. These pions and neutrons are very efficient at breaking up oxygen nuclei and produce isotopes. This is the dominant channel for isotope production.

Our theory explains the observed light-profile peaks — they are Cherenkov light from showers — and the observed correlations — showers make spallation backgrounds. However, we left out one problem: showers are only ∼5 m in size, whereas the observed peaks in Super-K are ∼30 m wide [26]. We addressed this problem in the next paper.

Chapter 4 is the third paper in the series. Here, we explain why the observed showers in Super-K are much larger than their true sizes, and how to use better reconstructed profiles for new cuts.

The majority of the paper involves careful simulation of Cherenkov light propagating in water, and how it gets detected on PMTs with finite timing and position resolutions. We realize that because the particles in showers are slightly deflected away from the primary muons, and hence their Cherenkov light is also deflected, the finite PMT timing resolution blows up. We then propose a method to reconstruct shower profiles that can deal with this problem and gives more faithful shower profiles. Finally, we propose a spallation cut that takes into account the fact that the isotope production probability is correlated with shower light intensity.

Chapter 5 is an independent paper, addressing high-energy astrophysical neutrino detection in IceCube, but it connects to the spallation work.

IceCube cannot distinguish between electron flavor neutrino and tau flavor neutrino because they both make cascade events (Sec. 1.2.1). However, if we look at the particle content of neutrino interactions, $\nu_e$-initiated showers are mostly electromagnetic and $\nu_\tau$-initiated showers are mostly hadronic. So, if we can find observables that are produced by the hadronic component of the showers, we should be able to distinguish $\nu_e$ and $\nu_\tau$ because the signals should be stronger in $\nu_\tau$ events.
Inspired by our studies of showers for Super-K, we realized that the pions (and the subsequent muons) and neutrons made in showers produce additional light signals when they decay or capture. These decays and captures occur well after the prompt shower; hence, we name them “muon echoes” and “neutron echoes”. The echoes are the collective light from many individual decays and captures, each emitting light in the MeV range. In this work, we use FLUKA to simulate the light intensity of collective muon decays and neutron captures, and conclude that although quite challenging, IceCube does have a good chance to observe them and, hence, to distinguish $\nu_e$ from $\nu_\tau$ interactions.
Chapter 2

First calculation of cosmic-ray muon spallation backgrounds for MeV astrophysical neutrino signals in Super-Kamiokande

When muons travel through matter, their energy losses lead to nuclear breakup ("spallation") processes. The delayed decays of unstable daughter nuclei produced by cosmic-ray muons are important backgrounds for low-energy astrophysical neutrino experiments, e.g., those seeking to detect solar neutrino or diffuse supernova neutrino background (DSNB) signals. Even though Super-Kamiokande has strong general cuts to reduce these spallation-induced backgrounds, the remaining rate before additional cuts for specific signals is much larger than the signal rates for kinetic energies of about 6 – 18 MeV. Surprisingly, there is no published calculation of the production and properties of these backgrounds in water, though there are such studies for scintillator. Using the simulation code FLUKA and theoretical insights, we detail how muons lose energy in water, produce secondary particles, how and where these secondaries produce isotopes, and the properties of the backgrounds from their decays. We reproduce Super-Kamiokande measurements of the total background to within a factor of 2, which is good given that the isotope yields vary by orders of magnitude and that some details of the experiment are unknown to us at this level. Our results break aggregate data into component isotopes, reveal their separate production mechanisms, and preserve correlations between them. We outline how to implement more effective background rejection techniques using this information. Reducing backgrounds in solar and DSNB studies by even a factor of a few could help lead to important new discoveries.

The contents of this chapter were published in Ref. [2].
2.1 Introduction

Neutrinos are powerful probes of the universe and its contents. They are abundantly produced by nuclear fusion processes that convert protons into neutrons, through the decays of unstable particles and nuclei created in high-energy processes, and through pair production in hot, dense environments. They can reach us unattenuated and undeflected from vast distances or from behind enormous column densities of matter, directly revealing the energies and timescales of the processes that made them. Even in a core-collapse supernova, where the neutrinos are thermalized by scattering, they emerge at energies $\sim 10$ MeV over about $10^3$ s, compared to photons, which emerge at energies $\sim 1$ eV over months. The detection of astrophysical neutrinos allows us to probe physical conditions and neutrino properties beyond the reach of laboratory experiments.

The first great challenge of neutrino astronomy is the fact that the small interaction cross sections that make the above possible make detection difficult. This can only be solved by brute force — building large enough detectors to ensure adequate event rates. We focus on Super-Kamiokande (Super-K), the world’s largest low-energy neutrino detector, which has a fiducial mass of 22.5 kton of water and a total mass of 50 kton of water [87, 88]. (For comparison, neutrinos were first detected in the Reines-Cowan reactor experiment with a detector using less than 1 ton of scintillator [89].) Even with such a large detector, the measured rates of low-energy astrophysical neutrinos are very small: about 15 solar neutrino events (all flavors of neutrinos elastically scattering electrons) detected per day [14, 24, 90] and an upper limit of several events (primarily $\bar{\nu}_e$ inverse beta decay) detected per year from the diffuse supernova neutrino background (DSNB) [26, 91–94].

The second and far greater challenge of neutrino astronomy is reducing detector backgrounds to isolate these rare signals. Immense care and sophistication is required, and continual progress with existing detectors is possible. The primary backgrounds for solar and DSNB signals are MeV electrons and positrons from the decays of nuclei and muons. Below about 6 MeV detected electron kinetic energy, intrinsic radioactivities are the dominant background in Super-K [14, 24, 25, 90], and these are controlled through the selection and purification of materials, choice of water circulation pattern to minimize radon ingress, and software processing (e.g., reconstruction quality and fiducial volume cuts). From about 6 to 18 MeV kinetic energy, induced radioactivities produced by cosmic-ray muons are the dominant background [14, 24, 25, 90], and there is great potential to reduce these with the help of theoretical work.

To reduce cosmic-ray backgrounds, Super-K was built under 1000 m of rock (2700 m water equivalent) in the Kamioka mine in Japan [87, 88]. As cosmic-ray particles interact with the rock and lose energy, their flux is reduced. The only high-energy particles that reach the Super-K detector are muons and neutrinos. The muon flux is $6.0 \times 10^5$ m$^{-2}$.
hr$^{-1}$ at sea level, and is reduced to 9.6 m$^{-2}$ hr$^{-1}$ at Super-K [95], which corresponds to a muon rate in the detector of about 2 Hz [14]. It is easy to veto the muons themselves, but they frequently produce relatively long-lived radioactive isotopes through the breakup ("spallation") of stable nuclei directly or, more commonly, through secondary particles produced through muon energy-loss processes. The spallation rate is large, $\sim 1$ interaction per through-going muon in Super-K, though many of the daughter nuclei are stable or decay in ways that do not produce Cherenkov signals.

Super-K has cuts to reduce backgrounds from the decays of spallation products, but these have to be limited to not overly discard signal events. Many of the unstable isotopes produced have half-lives of order 1 s, comparable to the time between successive muons. It is easy to estimate that a simple cut of all events in a cylinder of radius even a few meters around each muon track for a few seconds leads to a detector deadtime of $\sim 20\%$. The real algorithm used by Super-K is more complex, and is based on a likelihood analysis that takes into account distance and time from the preceding muon as well as a variable related to muon energy loss, but a similar deadtime is achieved [14, 96]. Even though the Super-K spallation cuts have a rejection efficiency of $\sim 90\%$ [25], the remaining background rate is still $\sim 10$ times greater than the solar neutrino signal rate above several MeV (this is then reduced by another factor $\sim 10$ by the solar direction cut, leaving a background comparable to the signal) [24]. For the DSNB search, a higher energy threshold can be used to dramatically reduce backgrounds, but spallation decays are still overwhelming below about 18 MeV [91] (16 MeV with new techniques [26]).

Our goal for this paper is to detail the production processes for spallation backgrounds in Super-K and the physical characteristics of where, when, and with what associated particles these decays occur. With this information, it will be possible to make better cuts to reject backgrounds while preserving signals. For solar neutrinos, such improvements could help improve the significance of the 2.7-$\sigma$ hint of the day-night effect from neutrino mixing in Earth [97–100]. They may also help lead to the first detection of the hep neutrino flux, which is likely only a factor of a few away from detection [14, 41, 101–103]. Such measurements would improve our knowledge of the Sun and of neutrino mixing parameters [9, 104, 105]. Reduction of spallation backgrounds would also help lower the energy threshold in the DSNB search [26, 91] to where the signal is larger [92, 93], which might help lead to a first detection.

Until now, there has been no detailed published study of spallation backgrounds in water. The Super-K cuts have been developed from empirical studies [14, 24, 26, 90], and not from theoretical calculations. Further, they treat all isotopes together, without taking into account significant differences in their production, properties, and distributions. With Super-K nearly reaching the sensitivity needed for the above discoveries, a more detailed approach is needed. The interactions of muons with scintillator have been studied
This paper is not meant to be a comprehensive study. It is a first step in understanding spallation backgrounds in water-based detectors, beginning with the yields and the average physical distributions of secondaries and isotopes. In two subsequent papers, we will go further, showing how characteristics of the showers of secondary particles that produce isotopes can be used to tailor better cuts [26] and how those would be improved if Super-K gained the ability to detect neutrons by adding dissolved gadolinium [115].

This paper is organized as follows. In Sec. 2.2, we describe the setup for our simulation. In Sec. 2.3, general points about muon energy loss and secondary particle production are discussed. Our main results are in Sec. 2.4, where we calculate the neutron and isotope yields and study the properties of the induced backgrounds. Finally, we present our conclusions in Sec. 2.5.

### 2.2 Setup of calculations

The Monte Carlo code FLUKA (version 2011.2b.3) [84, 85] is used for this work. It is a comprehensive code for particle energy loss and interactions with matter. For our purposes, FLUKA simulates all the physics processes relevant for the interactions of muons and their secondaries with water, including electromagnetic processes such as charged-particle ionization and bremsstrahlung, gamma-ray pair production and Compton scattering, and hadronic processes such as pion production and interactions, photo-disintegration, and low-energy neutron interactions with nuclei. It has been extensively used to simulate muon interactions in underground detectors, e.g., Refs. [82, 83, 95, 116–118]. The FLAIR interface [119] is used when running FLUKA.

Most of the relevant physics processes and libraries are included in the FLUKA defaults. To make the low-energy neutron treatment more straightforward, the PRECISIOOn card was chosen. Some muon processes, such as photo-nuclear and bremsstrahlung, were specifically activated. The new ion transport library was used.

The first main input for our simulation is the detector setup. The Super-K detector is a cylinder of water of diameter 39.3 m and height 41.4 m [14]. The outer detector (OD) is separated from the inner detector (ID) by a layer of photomultiplier tubes, most inward-facing, some outward-facing. The ID is about 2.5 m away from the edge of the detector [87, 88]. Our results are calculated only in the fiducial volume (FV) region, which is a virtual cylinder with each side 2 m away from the ID (and about 4.5 m from the outer edge of the OD), containing 22.5 kton of water [14]. Water is one of the FLUKA pre-defined
materials, including the natural abundances of hydrogen and oxygen isotopes. Muons may also interact with the surrounding rock to produce showers that enter the detector and produce isotopes. In the geometry setup, we include 2 m of rock outside the detector to induce secondary production (see Refs. [120, 121]), though it has only a modest effect.

The other main input for our simulation is the muon energy spectrum shown in Fig. 2.1. The curve is the simulated muon flux at Super-K [22]. Because the muon energy is plotted on a log scale, the flux is plotted as $E \frac{d\Phi}{dE} = 2.3^{-1} \frac{d\Phi}{d\log_{10}E}$, so that the integrated number of particles per decade (or other interval of fixed multiplicative width) is proportional to the value of this curve (i.e., plotting just $d\Phi/dE$ underweights the importance of high-energy bins). The two vertical lines indicate characteristic energies. The one near 6 GeV is the minimum ionization energy loss for muons passing vertically through Super-K. Muons with less energy stop in the detector (as shown in the figure, these are only $\sim 5\%$ of all muons). The line near 1000 GeV is the muon critical energy, at which the radiative energy loss equals the ionization energy loss. Muons with higher energies are more likely to produce showers, and thus more isotopes.

By number, most muons are in the range 30 – 700 GeV, with an average energy of 271 GeV [22]. The spectrum drops at high energies due to the falling spectrum of cosmic rays and at low energies due to muon energy loss in the rock above Super-K. Integration of the spectrum gives a muon rate at Super-K of 1.8 Hz [22], which is consistent with the published values of 2 – 3 Hz [25, 96, 122, 123]. Specifying the muon rate more precisely requires knowing unpublished details about the muon multiplicity, path length and angular distributions, and stopping fraction. Other studies have shown that the detailed shape of the spectrum, for the same average energy, does not affect the isotope yield much [82, 117].

We adopt several simplifications for the primary muons. All muons in our simulation are vertically down-going. In reality, most muons are down-going, but not perfectly [124]; Tang et al. [22] show that about 75% of muons have down-going zenith angle $\cos \theta > 0.5$ for KamLAND, which is at the same depth and location as Super-K. A complete 2D map of the simulated angular distribution of muons at Super-K is given in Ref. [22, 124]. Muons are sent only along the cylinder center. These two simplifications do not affect our results. Super-K has very good reconstruction for muon tracks, and all our secondary and isotope yields are calculated per muon path length. For muons coming in at an angle or a different spot, it would be easy to rescale our results by the actual muon track length. Besides single through-going muons, there are also muon bundles and muons that only go through a detector corner. We focus on single through-going muons, because they are the most common and because the other cases are easily identifiable. We simulate only $\mu^-$; there are also $\mu^+$, but the isotope yields from $\mu^-$ and $\mu^+$ differ very little [82, 83], except for nuclear captures of stopping $\mu^-$, which we discuss below.

A similar setup was adopted for the spallation study by KamLAND [82]. In their
Figure 2.1: Simulated cosmic-ray muon flux spectrum (integrated over angles) at Super-K [22]. The line near 6 GeV is the minimum ionization energy loss for a vertical muon passing through the Super-K FV. The line near 1000 GeV is the muon critical energy, above which radiative energy losses dominate. The fluctuations are from limited statistics in the simulation and are not significant.

study, spallation yields were measured experimentally and compared to simulation results from FLUKA. The Borexino spallation study [83] used both simulation packages FLUKA and GEANT4. Overall, it was found that there are factor of 2 discrepancies between the calculated yields and also between those and the measured values, which is reasonable, given the hadronic uncertainties and that yields for different isotopes vary by orders of magnitude.

2.3 Muon energy loss and secondary production

The average muon energy loss rate is [35, 125–128]

$$\frac{dE}{dx} = \alpha(E) + \beta(E)E.$$  \hspace{1cm} (2.1)

The $\alpha$ term corresponds to the continuous energy losses due to the ionization (and excitation) of atomic electrons. It has a typical value of 2 MeV cm$^2$ g$^{-1}$ and does not change much with muon energy. The ionization can be separated into a restricted ionization energy loss, which is the ionization with soft collisions and small fluctuations, and delta-ray production, which has hard collisions and large fluctuations [35]. The $\beta E$ term corresponds to the energy losses due to radiative processes through interactions with atomic nuclei. For muons at hundreds of GeV, pair production and bremsstrahlung are the most important radiative processes, while photo-nuclear has a small contribution [127]. Pair production is
a nearly continuous energy loss, but bremsstrahlung and photo-nuclear energy losses have large fluctuations. Ionization and radiation losses are equal at about 1000 GeV for muons in water, which defines the muon critical energy \( E_c \) [127].

Figure 2.2 shows the energy loss distribution for vertical (path length 32.2 m) through-going muons in the Super-K FV. The restricted ionization energy loss is about 6 GeV and the pair production loss is about 1 GeV. These two terms have almost no fluctuations and correspond to the minimum energy loss of 7 GeV shown in Fig. 2.2. On average, muons lose about 11 GeV, which means 4 GeV for the total of the delta-ray production, bremsstrahlung, and photo-nuclear processes. Bremsstrahlung energy loss is primarily responsible for producing the high energy loss tail [35].

Muons lose energy to the production of secondary particles, and there is a lot of energy available to make many of them, as shown in Fig. 2.2. These interactions do not appreciably affect the parent muon, as the energy loss in the detector is small compared to the muon energy. The muon interaction cross sections then do not change much as muons lose energy traveling through the detector [127]. The muon tracks have only minor deflections, with 90% of muons having less than 30 cm transverse displacement when they exit the FV.

Figure 2.3 shows the average production of secondaries by muons in Super-K. The plotted path length spectrum is the sum of distances traveled by all secondary particles of the same species at certain energy. It is similar to the particle multiplicity times the mean free path. The difference is that here a particle contributes to the path length at low energies after it travels some distance at high energies, so there is a pileup of path length

![Figure 2.2: Probability density function of calculated energy loss for vertical through-going muons passing through the Super-K fiducial volume (path length 32.2 m). The muon energy spectrum used is shown in Fig. 2.1.](image-url)
from high energy to low energy. This path length spectrum is the most useful quantity for calculating interactions by these particles. These results do not depend on density because they are calculated per muon path length (here the vertical distance through the Super-K FV).

As shown in Fig. 2.3, the dominant secondaries are gammas, followed by electrons (and positrons). This makes sense because the primary ways for muons to lose energy other than ionization are delta-ray production, pair production, and bremsstrahlung, all of which are electromagnetic. In Fig. 2.2, the average radiative muon energy loss is 5 GeV. The accumulated path length of the secondary electrons and positrons should be \( \sim \frac{5 \text{ GeV}}{0.2 \text{ GeV/m}} \sim 25 \text{ m} \), and the integral of their curve in Fig. 2.3 is close to this.

A similar figure in Ref. [95], which is based on independent calculations, shows secondaries produced by muon interactions in scintillator. Detailed comparison between Fig. 2.3 and Ref. [95] (taking into account the different plotting scales) shows consistent results. As expected, there is not much difference between muon interactions in water or scintillator for muon energies of hundreds of GeV. A minor discrepancy is that there are more \( \pi^+ \) than \( \pi^- \) in Fig. 2.3, whereas it is the opposite in Ref. [95]. To check this, we ran a separate simulation without hydrogen and found that the slight difference in our Fig. 2.3 between \( \pi^+ \) and \( \pi^- \) is due to scattering of \( \pi^- \) on free (hydrogen) protons. Our best guess is that the \( \pi^+ \) and \( \pi^- \) curves in the figure of Ref. [95] are mislabeled.

All of the results presented here are averaged over many muon path lengths. In fact, secondaries are made primarily in electromagnetic and hadronic showers, not uniformly along muon tracks. In our simulation runs, we see significant correlated variations in the muon energy loss, secondary production, and isotope production along the muon paths. This is hinted at by the high particle energies in Fig. 2.3. In our follow-up papers, we will discuss the shower nature of secondary production and how taking it into account can help improve background rejection in Super-K.

Muons interact with oxygen nuclei directly to produce isotopes, but the dominant mechanism to make isotopes is through secondaries breaking up oxygen nuclei. The most important secondaries in this regard are neutrons, pions, and gammas. Of all spallation-induced isotopes that cause backgrounds in Super-K, only 11% are made by muons (7% are \(^{16}\text{N}\) from stopping muons plus 4% other isotopes); the rest are made by secondary particles.

The physical distributions of the secondaries tell us where the isotopes are being made. The differences reflect how the different secondaries lose energy. Figure 2.4 shows the normalized distribution of secondary particle absorption distances to the muon track. The distribution is \( \text{d}N/\text{d}r \text{[cm}^{-1}] \), i.e., the area factor \( 2\pi r \text{d}r \) is included. Compared to Fig. 2.3, electrons (and protons) are not shown because they are not major parent particles for spallation products. The gammas have a short mean free path and are mostly forward. Most gammas are destroyed by pair production, and the Moliere radius (9.8 cm in water [35])
Figure 2.3: Secondary particle path length spectra made by cosmic-ray muons in Super-K. The y axis is the cumulative path length, i.e., the total distance traveled by all particles of a given species at each energy, and the x axis is kinetic energy. Here e means the sum of electrons and positrons. The proton path length is not shown; it is similar to the pion path length. The curve for low-energy secondary muons, also not shown, is at or below $10^{-3}$. The results are calculated per single muon path length, here the 32.2 m vertical distance in the FV (in contrast, in Table 2.1 below, the yields are quoted per cm of muon track, i.e., $\mu^{-1} \text{g}^{-1} \text{cm}^2$).

sets a scale for gamma distances from the muon. The mean free path for pions at these energies is about 1 m [35]. Assuming pions are destroyed after only one interaction (e.g., $\pi^-$ absorption on p), the falling distribution corresponds to a typical forward direction of $\cos \theta \sim 0.9$. This is consistent with Fig. 2.3, where most pions are relativistic. Among muon secondaries, neutrons travel the furthest from the muon track, with 98% of neutrons contained within 3 m. The neutron mean free path is $\sim 10$ cm above a few MeV, and less at lower energies; neutrons go much farther than this because many scatterings are required to stop them [129]. The result is very similar to the neutron distance distribution in scintillator [83]. The carbon number density in scintillator and the oxygen number density in water are comparable, but the cross section for neutrons on oxygen is slightly higher than that on carbon [130]. As a result, neutrons travel a bit less far in water. Compared to the average distance of 74 cm in water, the average distance in scintillator is 81.5 cm [83]. Most neutrons are absorbed by capture on hydrogen at non-relativistic energies; we also count the reactions of energetic neutrons on oxygen, e.g., (n,p), though this is a small effect. The Borexino [83] measurement counts only gamma-ray producing captures on hydrogen (mostly) and carbon.
2.4 Isotope and neutron production and distributions

Using the muon and secondary data, we calculate the isotope and neutron yields in Super-K using FLUKA. The isotope counts are read from the RESNUCLEi card. Neutron counts and production channels are taken from a modified mgdraw.f subroutine. For neutron counts, processes like (n, 2n) are carefully taken into account.

We began our study by reproducing all of the relevant KamLAND results [82], and extending the isotope yields to include stable isotopes for comparison to the yields of analogous (stable or unstable) nuclei in Super-K. Consistent results, within a factor of 2, validate our approach. The results show interesting differences in the physics of spallation in water and scintillator, as discussed in detail below.

2.4.1 Predicted Yields

Table 2.1 shows the neutron and isotope yields per muon along with associated details. Almost all isotopes made by muons and their secondaries are listed (we skip isotopes with small yields or small mass numbers). Since Super-K can only detect relativistic charged particles, only betas and gammas (through pair production or Compton scattering) can be seen, while decay products such as neutrons, protons, and alpha particles are invisible (neutron captures on protons are very hard to detect [94]). The top part of the table contains isotopes that β decay and thus are backgrounds in Super-K (referred to as background.
The bottom part of the table contains isotopes that are stable, have long half-lives, or decay invisibly.

The half-lives of the unstable isotopes range greatly, from 0.008 s to 13.8 s. A timescale to compare to is the average separation between muons, about 0.5 s. The beta decay spectra are complicated and have various branches. Here only the dominant decay modes are listed, though our calculations take all modes into account. Unsurprisingly, many of the spallation isotopes are short-lived and high-energy compared to intrinsic radioactivities. The half-lives and decay modes are taken from [131]. The isotope decay spectra are taken from Ref. [23] for $^{16}$N, Ref. [132] for $^{8}$B, and Ref. [133] for all other isotopes.

The fourth column shows the isotope yields calculated with FLUKA. These span five orders of magnitude, which is an important point. As noted, the accuracy of the isotope production rate is only about a factor of 2. Yet, because the yields among different isotopes are so different, we can still get a good understanding of their relative importance. Another point is that the production of beta-decaying isotopes is relatively rare. The sum of unstable isotopes is 58 in the units of the table, corresponding to about 0.02 unstable isotopes per muon (i.e., multiplying by the vertical distance of 3220 cm). The sum of the stable or invisible isotopes is around 2950, or about 0.9 isotopes per muon. Neutrons are produced with a yield comparable to that of all isotopes.

The current Super-K solar neutrino analysis has a kinetic energy threshold of 3.5 MeV [134], and taking this into account changes the importance of different isotopes. The fifth column shows the production rate of isotopes with decay energy larger than 3.5 MeV. Of unstable isotopes with high yields, $^{16}$N is cut the least. For $^{16}$N decay, 66% of the time there is a 6.1 MeV gamma ray, which leads to an electron-equivalent energy reduced by a factor $\sim 1/4$ [23]. As a result, the beta spectrum is shifted to higher energies, making it unaffected by the 3.5 MeV cut. The sum of the yields of background isotopes is reduced to 50 in the units of the table.

The last column shows the most important production channel for each isotope. For most isotopes, there are several production channels, with different parent particles, often of comparable importance. Statistically, the assignments of parent particles in the simulation are correct. For low energy neutrons ($E < 20$ MeV), FLUKA uses a multi-group treatment, so the correlations among daughter particles are not accurate. In cases where production by neutrons is important, the results provide a good first understanding, but are not accurate descriptions of the actual interactions.

The final states of the production channels for each isotope indicate particles that could possibly be detected in association with creation of the isotope. (In addition, there will frequently be prompt gamma rays from the de-excitation of daughter nuclei [135–138], but the Cherenkov light from their subsequent signals will be buried under that from the muon.) It may be possible to identify pion decays in some cases. Protons and alpha
particles will almost always be non-relativistic and hence non-detectable. At present, it is very difficult to detect neutrons in Super-K [94], though that would change with the addition of gadolinium [115]; neutron captures are prompt (about 200 \( \mu \text{s} \) in pure water and about 10 times shorter if gadolinium is added), so they are efficiently removed by even a short time cut following a muon. An important application could be identifying the production of \(^8\text{He}\) and \(^9\text{Li}\), the decays of which can mimic an astrophysical inverse beta signal because there is a beta followed by a neutron capture. We find that there is frequently a neutron produced in association with these isotopes, so there would be a neutron capture preceding the \(^8\text{He}\) or \(^9\text{Li}\) decay, unlike for a real astrophysical signal event. However, we caution that further study of the contributing channels is needed.

The production of \(^{16}\text{N}\) was independently calculated in Ref. [95]. This is the most abundant background isotope from muons and it has a long half-life. The dominant way to make \(^{16}\text{N}\) is \(^{16}\text{O}(n,p)^{16}\text{N}\), which has a yield of \(14 \times 10^{-7} \mu^{-1} \text{g}^{-1} \text{cm}^2\), to be compared to the value found by Ref. [95], \(23 \times 10^{-7} \mu^{-1} \text{g}^{-1} \text{cm}^2\). Sudbury Neutrino Observatory has an upper limit on the \(^{16}\text{N}\) yield of \((20-25) \times 10^{-7} \mu^{-1} \text{g}^{-1} \text{cm}^2\) [139]. All of these are consistent.

In our simulation, we consider only primary \(\mu^-\). Other studies have shown that isotope production by \(\mu^+\) and \(\mu^-\) typically differs by only a few percent [82]. One exception is stopping \(\mu^-\), which can capture on oxygen and make \(^{16}\text{N}\) by \(^{16}\text{O}(\mu^-\nu\mu)^{16}\text{N}\). Stopping \(\mu^-\) make \(\sim 17\%\) of \(^{16}\text{N}\), for which Super-K has a separate cut [14]. Consequently, if we take primary \(\mu^+\) into account, the \(^{16}\text{N}\) yield would change by about 8%. For most subsequent calculations and comparisons to Super-K measurements, we ignore the \(\mu^+\) correction to isotope production.

\subsection*{2.4.2 Comparison to Super-K Measurements}

In the following, we focus our comparisons on data above 6 MeV. At lower energies, detector backgrounds from intrinsic radioactivities are dominant. The largest intrinsic radioactivity background in the water itself is due to the \(^{214}\text{Bi}\) beta decay following \(^{222}\text{Rn}\) ingress; though its endpoint is 3.26 MeV, energy resolution smears the spectrum to higher energies [14, 24, 140] (see also Ref. [141]). There are also radioactivities in the photomultiplier and other detector elements, and these are largely reduced through the fiducial volume cut [14, 24]. This dividing line of 6 MeV is in good agreement with the demonstrated effectiveness of the spallation cut above this energy [14, 24, 90], as well as by the results of a dedicated spallation study [25].

Super-K has given a likelihood function of decay time \(t\) after the primary muon for decays in a cylinder around the muon path [14, 96]. This time is well defined because the muon takes only about 100 ns to cross the detector. The likelihood function is an empirical fit to the sum of all spallation backgrounds, and isotopes with similar half-lives are grouped together. With the simulated yields from FLUKA, we have each component of
Figure 2.5: Spallation decay rate distribution. The y axis is dimensionless, and the relative heights of each curve correctly show their relative contributions. The $^{16}$N decay spectrum is taken from Ref. [23] and the effects of the Super-K energy resolution [24] are included. **Left panel:** The blue line is our FLUKA results, compared to the Super-K empirical fit to spallation-selected data, both with a kinetic energy cut of $E > 6$ MeV. The total decay rate is normalized to the Super-K fit, which is measured with high statistics. The dashed lines show how some example isotopes contribute to the total rate. **Right panel:** The same, after a 10 MeV kinetic energy cut.

this separately.

Figure 2.5 (left panel) shows our combined spallation product decay rate compared to the Super-K fit. The normalization is chosen so that the integrated event numbers are the same between the simulation and the Super-K fit. Overall, the total decay rate and the Super-K fit agree well, up to a factor of 2. The four most abundant isotopes have very different half-lives. This figure shows how each contributes to the total decay rate on different timescales. Below about 0.1 s, $^{12}$B is dominant (with a smaller contribution from $^{12}$N, which has a comparable half-life and decay energy); between 0.1 s to 3 s, $^{8}$Li contributes most; and, after about 3 s, $^{16}$N is dominant. We also show $^{11}$Be, which has the longest half-life, 13.8 s. All of the curves in Fig. 2.5 (left panel) have a kinetic energy cut of 6 MeV.

Figure 2.5 (right panel) shows a similar result with a 10 MeV kinetic energy cut to the calculation (the similar Super-K measurement is not available). The main effect of the energy cut is to decrease $^{16}$N compared to other isotopes. A relatively high energy cut works well for $^{16}$N because of its low endpoint energy.

Another comparison we can make with Super-K results is the energy spectrum of spallation backgrounds in the FV. Similar to above, Super-K has the total decay energy spectrum
Figure 2.6: Spallation background energy spectra. The y axis unit is events per day in the Super-K FV in 0.5 MeV energy bins. Here the prediction is not normalized to the data. (In this figure, the expected solar neutrino signal after cuts is $\sim 1$ at low energies, $\sim 0.1$ at medium energies, and vanishing at high energies, as shown in Fig. 39 of Ref. [14].) **Left panel:** The thin blue line shows the total energy spectrum from our FLUKA results, adding up all the component isotope decay spectra, weighted with their yields (shown with dashed lines for some example component isotopes). The thick blue line is the total spectrum smoothed with the Super-K energy resolution [24]; the component spectra are shown before smoothing. The black stepped line shows the Super-K measurement of the total background spectrum before spallation cuts [25], which is measured with high statistics. For normalization, the Super-K FV muon rate of 1.88 Hz and the mean muon path length of 32.2 m are used. Gamma energies are not included in these spectra, as doing so would have only a small effect (it would matter most for $^{16}$N, but that is a subdominant component here). **Right panel:** The same, after a 0.3 s time cut.

from all background isotopes [25]. With the simulated yields, adding up the component spectra from all isotopes gives a total spectrum that can be compared to data.

Figure 2.6 (left panel) shows that the simulation and the measurement agree quite well above 6 MeV. For this comparison, the isotope yields were multiplied by the average muon rate at Super-K (1.88 Hz) and the average muon track length in the FV (32.2 m). Both numbers have uncertainties because we do not know the precise definitions used by Super-K. This, together with the limitations of the simulation, introduce the biggest uncertainties. Taking energy resolution into account is important: the high energy events seen in the detector are mainly from imperfectly reconstructed lower energy events. The agreement validates our results, especially because the absolute scale is predicted, not fit.

Figure 2.6 (right panel) shows the isotope spectra after a $t > 0.3$ s cut, which is about an order of magnitude less than our estimate of the time needed for a simple cylinder
cut around each muon (see Sec. 2.1). This is chosen to be short enough to not introduce significant deadtime and long enough to eliminate many short-lived isotopes. The total spectrum decreases by about a factor of 2. It also affects the relative contributions of isotopes at different energies. The dominant component at high energy without a time cut is $^{12}$N; after 0.3 s time cut, it is $^{8}$B. The fewer isotopes that contribute, the more effective isotope-specific cuts will be (see below).

The Super-K DSNB analysis of Ref. [91] has a lower energy threshold of 18 MeV total energy. The total background rate is $\sim 0.2$ events per day in the 18 – 20 MeV energy bin. The rate in Fig. 2.6 is consistent because the measured data in Ref. [91] include an increasing contribution from the decays of invisible muons.

The Super-K $^{16}$N calibration study reports that the production rate of $^{16}$N by stopping muons is 11 per day in an 11.5 kton volume [23]. The rate from our calculation is $3 \times 10^{-7} \mu^{-1} \text{g}^{-1} \text{cm}^{2}$. Taking into account the $\mu^{-}$ fraction in primary muons and the detector efficiency, we predict 22 events per day. The origin of the discrepancy is unknown, but the Super-K study reported problems with their measurement [23], so we view this factor of 2 as adequate agreement.

The fact that our same FLUKA predictions match both the energy spectrum and the time profile of the Super-K data is a powerful indication that they are accurate. In the energy spectrum, the components are largely overlapping because of the width of the beta spectra and the effects of energy resolution smearing. In the time profile, the components are better separated because of the wide range of half-lives. In combination, these provide strong tests of both the overall production rate of spallation products and the amplitudes of the many components.

### 2.4.3 Comparison to Yields in Scintillator

A major difference between spallation in scintillator and water is in the absolute background isotope yield. It is $\sim 0.3$ of the neutron yield in scintillator, whereas it is only $\sim 0.03$ of the neutron yield in water. (In scintillator and water, the neutron yields are similar to each other.) The reason is that there is a greater fraction of stable or invisibly decaying isotopes produced by muons in water. The neutron number is comparable to the total yield of all isotopes, both in scintillator and water. It is about 0.7 neutron per muon in the Super-K FV.

The production channels allow us to understand the different spallation processes better. The isotope yields between scintillator and water are similar if the production mechanisms are similar. Some of the most abundant isotopes are made by the ($\gamma$,n) reaction, which corresponds to $^{15}$O in water and $^{11}$C in scintillator. They have yields of 351 and 416 [82] in the units of $10^{-7} \mu^{-1} \text{g}^{-1} \text{cm}^{2}$. Luckily, $^{15}$O has a low beta-decay energy; in scintillator, $^{11}$C is a serious background. The most abundant background isotope in water is $^{16}$N, which
corresponds to $^{12}$B in scintillator, which has a comparable yield for the same muon path length.

2.4.4 Parent Particle Energy Spectrum

To understand isotope production mechanisms in more detail, we look at the energy spectra for secondaries making isotopes. Figure 2.7 (left panel) shows the spectra of parent particles of spallation background isotopes in Super-K. Here the y axis is a histogram of event number per MeV with arbitrary absolute normalization. The relative height reflects how important each parent particle is.

For making spallation backgrounds in Super-K, the most important parent particle is the neutron, as it contributes almost 10 times more than any others. The shape of the spectrum is a convolution of the neutron path length shown in Fig. 2.3 and the neutron-nucleus cross section. The peak below 20 MeV comes from the $(n, p)$ cross section [95]. Due to the nuclear capture of $\pi^-$ at rest, there is also a huge peak for low energy $\pi^-$. Gamma, $\pi^+$, and high energy $\pi^-$ contribute roughly equally, each only about half as much as the first $\pi^-$ bin. The parent particles of fast neutrons are similar to those for isotopes. Wang et al. [116] showed that at $E_\mu = 270$ GeV, most neutrons are produced by $\pi^-$, followed by gamma and neutron.

One interesting feature is that, even though the dominant secondaries produced directly
by muons are gammas and electrons, the ones that make background isotopes in water are mainly hadrons. This is consistent with the primary processes shown in Table 2.1. The fact that the gamma and pion curves initially rise with energy is consistent with the path length spectra in Fig. 2.3. The fact that these curves continue to high energies indicates the importance of showers for isotope production.

As discussed above, the result is somewhat different from muon spallation in scintillator. A rough count from the KamLAND result tells us that the main parent particle to produce isotopes is gamma, as it is responsible for $^{11}\text{C}$ and $^{7}\text{Be}$ production. This is consistent with the result shown in Fig. 2.7 (right panel). Here we show the parent particle spectra for all isotopes produced in water, including the stable ones and those that decay invisibly. The gamma contribution is significant, comparable to that of the neutron. Also, the relative height between the two panels shows the fraction of isotopes that are dangerous in Super-K relative to all isotopes. The reason for the big difference between the left and right panels is simply that in water, some of the most abundant isotopes made by gammas, e.g., $^{15}\text{O}$, $^{15}\text{N}$, and $^{12}\text{C}$, are invisible in Super-K.

### 2.4.5 Spatial Distribution of Isotopes

Because spallation products are produced by muons and their secondary particles, there are spatial and temporal correlations between spallation events and the parent muons. The muon itself emits Cherenkov light along its entire path, which makes it easy to detect. Thus, the correlations between muons and isotopes provide an opportunity for physics-motivated cuts.

There are two distances to describe the position of the isotope to the parent muon. One is the perpendicular distance to muon track, which is one of the variables for the Super-K likelihood function for the spallation cut. The other is the isotope position along the muon track.

Once isotopes are produced, they do not move far before they decay. Ions stop in a short distance, and there is no significant bulk motion of the water [88]. This can be seen from the fact that the Super-K likelihood function of isotope distance to the muon track shows a peak at very small distance [14]. Figure 2.8 shows our calculated distribution of isotope distance to the muon track. This shows one of the likelihood functions used for the Super-K spallation cuts. Our results are consistent with those shown in Ref. [96] (the Super-K results depend on a variable associated with muon energy loss; we summed over those distributions with appropriate weights). We did not take the Super-K position resolution into account in Fig. 2.8; it is about 1 m at 5 MeV and about 0.5 m at 10 MeV [24]. We find that 99% of isotopes decay within 3 m.

Each isotope has a different distribution, and we show two examples. The most abundant background isotope is $^{16}\text{N}$, and it dominates the low-energy end of the spectrum. On the
Figure 2.8: Cumulative distribution of isotope perpendicular distance to the muon track. The line marked “total” is for all isotopes, and the other curves are example isotopes.

other hand, $^8$B contributes the most at the high-energy end, as shown in Fig. 2.6. These two isotopes have quite different distributions. The 90% containment distance for $^8$B is 1.7 times smaller than that for $^{16}$N, which corresponds to a factor of 3 in cylinder volume. Taking this into account could improve cuts and reduce deadtime. For example, at high decay energies, $^8$B but not $^{16}$N can contribute, so a more specific cut could be used.

Figure 2.8 shows useful features for improving the Super-K likelihood function for the spallation cut. In the Super-K current likelihood function, the isotope distance to the muon track is one variable. However, the distance distribution for each isotope can be appreciably different. As a result, instead of using a combined likelihood function for all background isotopes, a likelihood function for each isotope separately should give a much more accurate description of the physics.

If we consider the isotope distance along the muon track, to first order we would expect a flat distribution when we average over muons (for individual muons, this would have bumps due to showers). The reason is that, on average, muons have hundreds of GeV energy and lose only about 11 GeV during propagation through Super-K. More precisely, the isotope yields decrease smoothly from the top of FV to the bottom of FV by several percent. This is partly due to the decrease of muon energy, and partly due to stopping muons. There is negligible spillover from the rock above Super-K.
2.5 Conclusions and Future Work

Guided by theoretical understanding and analysis, we use the simulation package FLUKA to study muon interactions with water, the production and properties of secondary particles, and the production and decay of unstable isotopes. Where possible, we compare our results to published measurements from Super-K, finding good agreement on an absolute scale, i.e., a factor of 2, which is reasonable considering the orders of magnitude differences in production rates. The residual discrepancies primarily arise from uncertainties in hadronic interactions and unpublished details of the muon backgrounds, and some of the differences could be reduced by calibration to measured data.

As a check, we also performed similar calculations for scintillator-based detectors, for which there are more extensive theoretical studies and experimental measurements. We focus on comparison to isotope and neutron production in KamLAND [82] and Borexino [83], finding good agreement, within the factors of 2 that have been noted by others between the measurements and calculations and also between calculations with FLUKA versus GEANT4 [116, 117].

One interesting point for context is how different the spallation backgrounds are in water Cherenkov detectors compared to scintillator detectors. First, for water there is the fortunate point that, although the production rate of all isotopes is comparable to that in scintillator, that of unstable isotopes is about ten times less. Second, many of the unstable isotopes decay without producing Cherenkov light. Scintillator detectors have the ability to detect neutrons through their radiative captures, and this is a significant advantage in identifying spallation products. However, if Super-K adds dissolved gadolinium to enable the detection of neutron captures, it will have a similar capability [115].

Our calculations for Super-K lead to important new high-level results beyond the details presented here. First, a demonstration that a theoretical calculation of the spallation backgrounds in water is now possible, even though it was not when Super-K began [96]. Compared to an empirical approach, production mechanisms are revealed, aggregates are separated into components, and correlations are preserved. Second, we show details that were heretofore unavailable. Important examples are differences between the distributions and correlations of each isotope, including temporal distribution after the muon, distance distribution away from the muon, decay energy spectrum, and associated particles.

We demonstrate that there is more information to be gained by having likelihood functions of time and distance for each isotope. Instead of a global likelihood for all spallation decays, our results could be used to construct per-isotope likelihoods that would lead to more precise cuts. Also, a new variable of decay energy can be used in addition to its original three variables of decay distance to the muon track, decay time, and muon energy loss. Even modest improvements, say a factor of a few, could lead to significant gains in the
ability to measure signals. This could help lead to first discoveries of the day-night effect and the hep flux in solar neutrinos, as well as the DSNB.

Our results are calculated for Super-K, but they could have wider applicability. The isotope yields per muon vary only moderately with depth, once that depth is appreciable, because they have a modest dependence on the muon average energy, scaling roughly as $E_{\mu}^{0.8-1.1}$ [82]. As first estimates, our results would provide useful comparisons for the Sudbury Neutrino Observatory [141], Hyper-Kamiokande [142], and the water shields of a variety of neutrino and dark matter detectors.

It would be valuable for Super-K to produce a dedicated study on spallation backgrounds informed by the predictions of this paper. The yields of different isotopes could be identified by a global fit that takes into account the full energy and time information on spallation decays, e.g., energy spectra in different time ranges, as has been done for scintillator detectors [82, 83]. Another key observable is the radial distributions of isotopes produced by different types of secondaries. An improved FLUKA simulation could be developed using a more complete description of the detector details, especially the muon distributions. It seems likely that the uncertainties could be reduced to well below a factor of 2 by calibrating the simulation to measured data.

It would also be valuable to have a similar study for the Sudbury Neutrino Observatory [141]. The very low muon rate and intrinsic radioactivities would make it easier to identify spallation decays and to avoid confusion over which muon was the parent. In addition, the ability to detect neutrons would help identify isotope production channels. With corrections for the different muon spectrum, detector properties, and the production of neutrons by deuterium photo-disintegration, it would be straightforward to relate these measurements to Super-K results.

In two follow-up papers, we will develop further ways to reduce backgrounds in Super-K and other water Cherenkov detectors. In the first paper, we will study the variations in muon energy loss along the path due to showers, and how this can be used to identify where isotopes are produced. This effect was discovered empirically in Ref. [26], and our results will provide the first detailed explanation of how it works and how it could be improved.

In the second paper, we will show how the ability to detect neutrons using gadolinium in water, as first suggested in Ref. [115], can be used to improve cuts to reduce spallation backgrounds. These papers will include some surprises that will allow significant gains in sensitivity beyond those enabled by results given here.

Acknowledgments

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Mosteiro, Masayuki Nakahata, Kenny Ng, Itaru Shimizu, Michael Smy, Mark Vagins, and Lindley Winslow for helpful discussions.
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Table 2.1: Table of simulated isotope yields. The top part has background isotopes for Super-K. The bottom part has isotopes that do not cause backgrounds in Super-K, including those that are stable, have long half-lives, or decay invisibly or with a low beta energy. For the 5th column, the Super-K energy resolution has been taken into account, though it makes little difference. The observed \(^{16}\text{N}\) decay spectrum (including both betas and gammas) is taken from Ref. [23]. For other isotope decays, only beta energies are included (gammas are ignored). Isotopes with yields smaller than \(0.01 \times 10^{-7} \mu^{-1}g^{-1}cm^2\) or \(A < 8\) (all of which are not backgrounds in Super-K) are ignored.
Table 2.1 continued

<p>| | | | | |</p>
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<td>38</td>
<td>(n,2α)</td>
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sum 3015 50
Crucial questions about solar and supernova neutrinos remain unanswered. Super-Kamiokande has the exposure needed for progress, but detector backgrounds are a limiting factor. A leading component is the beta decays of isotopes produced by cosmic-ray muons and their secondaries, which initiate nuclear spallation reactions. Cuts of events after and surrounding muon tracks reduce this spallation decay background by $\approx 90\%$ (at a cost of $\approx 20\%$ deadtime), but its rate at 6–18 MeV is still dominant. A better way to cut this background was suggested in a Super-Kamiokande paper [Bays et al., Phys. Rev. D 85, 052007 (2012)] on a search for the diffuse supernova neutrino background. They found that spallation decays above 16 MeV were preceded near the same location by a peak in the apparent Cherenkov light profile from the muon; a more aggressive cut was applied to a limited section of the muon track, leading to decreased background without increased deadtime. We put their empirical discovery on a firm theoretical foundation. We show that almost all spallation decay isotopes are produced by muon-induced showers and that these showers are rare enough and energetic enough to be identifiable. This is the first such demonstration for any detector. We detail how the physics of showers explains the peak in the muon Cherenkov light profile and other Super-K observations. Our results provide a physical basis for practical improvements in background rejection that will benefit multiple studies. For solar neutrinos, in particular, it should be possible to dramatically reduce backgrounds at energies as low as 6 MeV.

The contents of this chapter were published in Ref. [3].

3.1 Introduction

Neutrino astronomy in the MeV range has been very successful. Measurements of solar neutrinos confirmed many aspects of the nuclear fusion reactions that power the Sun; they
also provided essential information about neutrino mass and mixing, especially the matter-
induced effects. The detection of neutrinos from SN 1987A and the identification of its
progenitor star together confirmed the prediction that Type II supernovae arise from the
collapse of the core of a massive star into a proto-neutron star; the extreme conditions
allowed many novel tests of neutrino properties.

However, there are unresolved questions about the Sun and supernovae that can only
be answered with improved sensitivity. A better measurement of $^{8}$B neutrinos could im-
prove knowledge of the solar core temperature, test the energy dependence of the electron-
neutrino survival probability, and strengthen the signal of the day-night effect (presently
3 $\sigma$ [99, 100]) [105, 143–145]. A first detection of the hep flux would provide new tests
of the solar model and neutrino mixing. An eventual Milky Way supernova will allow
high-statistics tests of the physical conditions attending neutron-star birth, flavor mixing in
extreme conditions, and possibly black hole formation [146–150]. An immediate goal is the
first detection of the diffuse supernova neutrino background (DSNB), which will provide
new insights about supernova neutrino emission and the cosmic star formation history [93].

Discoveries could be made with existing experiments if detector backgrounds were re-
duced. We focus on Super-Kamiokande (Super-K), by far the largest low-energy neutrino
detector, with 22.5 kton of pure water in its fiducial volume (FV) [87, 88]. Great success
in reducing backgrounds has already been achieved, but further gains have been stubborn.
For the robustly detected solar-neutrino signal, the signal/background ratio is only $\sim 0.1$
after standard cuts; at forward angles relative to the Sun, the ratio is $\sim 1$ [14, 24, 90]. For
the DSNB search, the high background rate means that the analysis energy threshold is
above the peak energy of the signal spectrum [26, 91, 94]. Decreasing the background rate
by a factor $\gtrsim 10$ would substantially advance solar neutrino studies and the DSNB search.
Is this possible without building a bigger, deeper detector? Yes.

After standard cuts, the dominant background in the Super-K FV between 6–18 MeV is
beta decays of nuclear spallation products [14, 24, 25, 90, 96], which are short-lived isotopes
produced from oxygen in association with cosmic-ray muons. (At lower energies, longer-
lived isotopes produced through radon ingress and decay are dominant.) When a muon
passes through Super-K, a cut around the measured position of the muon track is made to
reject the spallation decays that follow; a difficulty is that some decay lifetimes are long
(up to 20 s; see Table I in Ref. [2]) compared to the average time between muons ($\sim 0.5$ s).
More precisely, a likelihood method is used to test events based on time elapsed since the
muon, distance from the track, and a variable related to muon energy loss. The empirical
cut that Super-K has developed for solar neutrino studies effectively removes $\sim 90\%$ of the
backgrounds but introduces $\sim 20\%$ deadtime, making it hard to improve.

In a previous paper [2], we performed the first theoretical calculation of the production
and properties of the spallation decay backgrounds for water-based Cherenkov detectors
such as Super-K. Our predictions are in good agreement, within a factor of 2, with Super-K data on the energy spectrum and time profile for the sum of spallation decay isotopes, and could be improved by calibration and more careful comparison. (Comparable accuracy is found in spallation studies for scintillator detectors [82, 83].) We detailed the physical processes behind isotope production and ways to use this knowledge to improve cuts. An important point is that nearly all isotopes are produced not by the muons themselves, but by the secondary particles associated with their energy-loss processes. At the depth of Super-K (2700 m water equivalent), where the average muon energy is 270 GeV, the average energy loss for a vertical throughgoing muon is 11 GeV, of which 7 GeV is from continuous processes such as ionization and 4 GeV from radiative processes such as delta-ray production and bremsstrahlung. Fluctuations can make the radiative losses much larger.

A recent Super-K paper on the DSNB search [26] showed that the Cherenkov light yield associated with a muon varies along its track, exceeding that expected for a single muon and presenting a broad peak (comparable in length to the height of the FV), and that subsequent spallation decays are correlated in position with this peak. The reasons for this variation, its properties, and its association with spallation decays went unexplained. However, it was found that these facts could be exploited to improve the rejection of spallation decays. Using an effectively shorter section of the muon track, several times less than the height of the FV, a more aggressive cut was used while keeping the deadtime moderate. This allowed Super-K to lower the analysis threshold for the DSNB search from 18 to 16 MeV, with zero spallation events remaining.

Here we provide the first explanation of the physics behind the Super-K technique, as well as new insights to substantially improve its effectiveness. Because the Cherenkov intensity (light emitted per unit length) of a relativistic muon is constant, the extra light and its variation must be due to additional charged particles, and a natural explanation is that these are produced in showers. However, the variations shown by Super-K (Fig. 2 in Ref. [26]) and Fig. 4.2 in Ref. [151] appear to be grossly inconsistent with this explanation, because the spatial extent is too large and the amplitude too small. Nevertheless, we find that the excess light is indeed due to particles in showers; that these showers are of short extent with high light intensity but appear long with low intensity due to Cherenkov reconstruction issues; that the correlation between the light profile peak and spallation production is because nearly all isotopes are made in showers; and that these reconstructions can be improved. Using our results, Super-K could refine their new cut down to 6 MeV to improve solar neutrino and DSNB studies.

The framework for our calculations closely follows that of our previous paper, and details are given there [2]. We use the particle transport code FLUKA [84, 85] (version 2011.2b.6) for our calculations, which has been used extensively for simulating muon-induced backgrounds in underground detectors [82, 83, 95, 116–118, 121, 152, 153]. We use the same
physics choices for FLUKA, details of the Super-K geometry setup, and the muon spectrum. Our calculations are for single throughgoing muons traveling 32.2 m vertically down the center of the FV. We assume that the positions of muon tracks are always well determined by a combination of outer-detector and inner-detector information, aided by the long lever arm of the muon track. For nonvertical throughgoing muons with shorter path lengths or for muon bundles, our results could be adjusted appropriately. We discuss stopping muons separately.

Whereas our previous paper considered the average behavior of muons (from one to the next, and along each track), we now follow the energy-loss variations of individual muons. We separately simulate how muons create daughter particles, how these daughters induce showers, and how these showers produce isotopes. With our new approach, we recover our previous results. All particles eventually produced following a muon are called secondaries; those in the first generation are called daughters.

The scope of this work is defined by a few choices. We focus on explaining and extending the results of Ref. [26]. We explain just the main features of the Super-K results; improving the details would require further input from them. We do not yet attempt a full calculation of the reduction in backgrounds; our estimates are enough to show the promise of new techniques. In our next paper, we will show why the Super-K Cherenkov reconstruction results appear to be inconsistent with showers and how they can be improved.

The remainder of this paper is organized as follows. In Sec. 3.2, we focus on the physics of showers — the energy spectra of their secondaries, their geometric properties, and the rates of showers as a function of their energy — to highlight physics insights critical to understanding later results. In Sec. 3.3, we detail how isotopes are produced and how this explains the observed correlation between Cherenkov light yield and spallation decays. Finally, we conclude in Sec. 3.4.

3.2 Shower Physics

Particle shower (or cascade) processes are central to this paper. Showers can be produced by radiative energy losses of cosmic-ray muons in Super-K, especially at high energies. The basic physics is that particles multiply in number through repeated interactions, with the particle energy decreasing in each generation. This continues until the average energy drops below a critical energy $E_c$ that depends on the type of shower and the medium. Below this, charged particles mostly lose energy by ionization.

For electromagnetic showers, the main secondary particles are electrons, positrons, and gamma rays. The dominant interactions in water are electrons and positrons producing gamma rays through bremsstrahlung with nuclei, and gamma rays pair-producing electrons and positrons, also with nuclei.
For hadronic showers, the main secondary particles are charged and neutral pions. Hadron interactions with nucleons produce pions, and pion interactions with nucleons can change both of their charges. The basic processes in electromagnetic showers leave the target nuclei largely intact, but that is not true for hadronic showers, which brings additional complications.

Figure 3.1 shows a typical shower. Shower lengths are around a few meters; shower widths are around tens of centimeters. Most electrons and positrons in showers are forward, with $\langle \cos \theta_z \rangle \simeq 0.9$. Showers are defined most generally by the phase-space density of their secondary particles, i.e., the joint number density in momentum and position, with time as a parameter. To express the cumulative effects of a shower, integrated over time, we use not the number density of secondary particles, which is only defined at a given instant, but rather some measure of their integrated effects. For a Cherenkov detector, it is useful to weight by path length; for charged particles, this is proportional to the light produced (and, especially for electrons, is nearly proportional to the energy deposited). Different integrals of the phase-space density are convenient for different purposes. The path length profile in longitudinal position (integrating over momenta and lateral positions) is probably the most familiar, and it determines the observable muon light profile in Super-K. The path length spectrum in energy (integrating over positions and the momentum directions) is not commonly shown, but it determines isotope production in Super-K. We present these in the opposite order, covering path length spectra in Sec. 3.2.1 and 3.2.2 and longitudinal profiles in Sec. 3.2.3.
To provide more detail on path length spectra, dL/dE describes the sum of distances traveled by all particles of a given species at each energy. This is obtained by integrating over the positions of the particles, and is called the volume-integrated fluence in FLUKA [2, 84, 154]. This spectrum multiplied by the cross section as a function of energy is the integrand for calculating the interaction rate. The integrated path length above the Cherenkov threshold determines the total Cherenkov intensity and thus the number of photomultiplier tube hits.

Super-K, a water-based Cherenkov detector, directly observes only relativistic charged particles. We focus on the light produced by showers induced by muons. The muons themselves produce Cherenkov light at constant intensity along the muon track [155]. Super-K cannot separate electrons from positrons or π− from π+, so, hereafter, electrons means the sum of electrons and positrons and pions means the sum of π− and π+, unless specified otherwise. Charged particles below their Cherenkov thresholds (kinetic energy 0.257 MeV for electrons and 70.1 MeV for pions [96]) are not detectable. Gamma rays and neutrons are not detectable directly, but only through their interactions.

We do not discuss isotope production by showers in this section. However, it is helpful to keep in mind that the most important parent particles for background isotopes are neutrons and pions; gamma rays make a small fraction of isotopes and electrons do not make isotopes [2]. Hence, even though neutrons, pions, and gamma rays contribute negligibly to Cherenkov light production, we discuss their behavior in showers.

In the remainder of this section, we first study the physics of showers in water independent of primary muons. Then we discuss how cosmic-ray muons make daughter particles and thus showers with a variety of energies in Super-K.

### 3.2.1 Electromagnetic shower spectra

Some important aspects of electromagnetic showers can be understood using simple principles. In a model proposed by Heitler [156], it is assumed that bremsstrahlung and pair production have the same mean free path (radiation length X₀), that this is energy independent, and that all other interactions, including electron ionization, can be ignored. Further, it is assumed that in each generation, particles travel the same fixed distance (d = X₀ ln 2) before they split into two particles, each with half the parent particle energy.

Figure 3.2 illustrates this process. If the shower starts with one particle of energy E₀, then after n generations, there are 2ⁿ secondary particles, each with energy

\[ E_n = \frac{E_0}{2^n} . \]  

(3.1)

The shower stops growing when the average particle energy is below the critical energy \( E_c \), which is set by the electron ionization energy loss in one radiation length [35]. Then, a
Figure 3.2: Schematic diagram of Heitler’s model for electromagnetic showers in the growing phase, which continues until the particle energies are below $E_c$.

shower reaches its maximum, where the number of particles is the greatest, after $\log_2(E_0/E_c)$
generations. Because the particles are mostly forward due to being relativistic, the distance
to the shower maximum is

$$
\ell = d \log_2 \left( \frac{E_0}{E_c} \right) = X_0 \ln \left( \frac{E_0}{E_c} \right). \tag{3.2}
$$

In water, $X_0 = 36$ cm and $E_c = 80$ MeV [35]. Electrons with energy $E_c$ lose all of their
energy by ionization in one radiation length. After shower maximum, gamma rays and the
electrons they scatter will travel somewhat further (a few radiation lengths). For a 10 GeV
shower, the longitudinal extent of a shower would be $\sim 2$ m, far less than the height of
Super-K. The true shower extent is greater than this, but not much, and is discussed in
Sec. 3.2.3.

Further properties of showers can be obtained analytically with more complex mod-
elss [157–163]. An example of the latter is the work by Rossi and Greisen [159], where they
derived results by solving the Boltzmann equations under certain assumptions. In their
Approximation A, which is only valid for high particle energies, asymptotic cross sections
for bremsstrahlung and pair production are assumed and electron ionization energy loss is
neglected. For the electron path length spectrum in an electron-initiated shower, they find

$$
\frac{dL}{dE} = 0.437 X_0 \frac{E_0}{E^2} \tag{3.3}
$$

for electron energies $E \gg E_c$. For electrons with energy greater than $E$, the distance to
Figure 3.3: Electron, gamma ray and pion path length spectra in terms of kinetic energy for showers initiated by electrons of energy $E_0 = 0.1, 1, 10,$ and $100$ GeV. The features seen at the injection energy arise because the showers have not yet reached an equilibrium mixture of $e^−, e^+, \text{and } \gamma$. The gamma-ray path length is shown only for $E_0 = 100$ GeV; the other cases are similar, except for having lower endpoints. The pion path length spectra are shown for $E_0 = 1, 10, \text{and } 100$ GeV (it is zero for 0.1 GeV). All spectra are normalized by $E_0$.

Their maximum is

$$\ell = 1.01X_0 \left( \ln \left( \frac{E_0}{E} \right) - 1 \right).$$  \hspace{1cm} (3.4)

This is similar to the Heitler result if Eq. (3.4) is (inappropriately) evaluated at $E_c$.

Contemporary work on showers is based on Monte Carlo simulation of all microscopic processes [164–167]. The fluctuations (distance, energy, etc.) in every interaction are taken into account, instead of solving for the average behavior with the Boltzmann equation. This enables the study of individual showers, as well as the variations among them. The simulation results are valid for the entire energy range, and the precision is excellent. In the following, we use theoretical insights to illustrate the physics behind our numerical results.

Figure 3.3 shows particle path length spectra for electron-initiated showers. We inject electrons with fixed energies into the Super-K FV, which is large enough to contain all secondary particles. We discuss Fig. 3.3 from high to low energy. As individual showers develop, the average energy of the shower particles decreases. At the peak, which is somewhat below $E_c$, the particle number is at a maximum. At lower energies, particles stop multiplying and the path length decreases due to particle ionization losses.

The way these and other results are shown is designed to highlight key physics points. As discussed, the numerator is the total path length traveled by a group of particles, and
not just the number of particles. We divide by the injection energy $E_0$ to show when there is universality (more energetic showers being just multiples of less energetic showers) or deviations from that. Because of the large range of energies, we use a log scale on the $x$ axis; also, this is especially appropriate for the showering phase, where particle energies change by factors, not shifts, between each generation. To calculate integrals of the curves, one should use $\log_{10} E$ as the integration variable. To match this choice of axis, we take derivatives with respect to $\log_{10} E$, which makes the height of the curve proportional to its importance in the integral; note that $dL/d\log_{10} E = 2.3 EdL/dE$ (see Ref. [2, 168] for further discussion). All energies in logarithms are in GeV units. A log scale is often used on the $y$ axis. This is of no particular importance, except that one should judge the relative contributions to the integral by numerical, not visual, height.

The spectra at high energies, during the shower phase, go as $dL/d\log_{10} E \sim 1/E$ for both electrons and gamma rays. The differential cross sections for bremsstrahlung and pair production can be factorized to roughly depend only on the fractional energy of the outgoing particles [35]. The path length spectra should be a function of $E/E_0$, and a power law shows this scale invariance [162]. The shower is extensive in (proportional to) $E_0$, so the length must be proportional to $E_0$. The result must also scale linearly with the radiation length $X_0$. Then, using simple dimensional analysis, we know the path length spectrum must scale as $\sim X_0 E_0/E^2$. This is consistent with the results of Rossi and Greisen [159]. The slight difference between the gamma-ray and electron path lengths at high energies in Fig. 3.3 is due to electron ionization, which matters more as the energy decreases.

The electron path length spectra at low energies, during the ionization phase, go as $\sim E^{0.5}$. To first order, ionization conserves particle number, but dissipates energy in the shower, so we might expect $dL/dE \sim$ constant and $dL/d\log_{10} E \sim E$. However, below the peak, there are many gamma rays from bremsstrahlung, as shown in Fig. 3.3, and these inject energy to electrons from the medium through Compton scattering. The competition between this and ionization produces the electron spectrum shown, including shifting the peak to an energy below $E_c$.

For an injection energy of 0.1 GeV or lower, showers do not typically develop. Electrons range out by ionization and do not produce or accelerate other particles. Gamma rays undergo Compton scattering and pair production, but they do not produce particles other than electrons.

The hadronic particle content in electromagnetic showers is quite small on average, and the pion path lengths are a few orders of magnitude less than those for electrons. The shapes of the pion spectra reflect the large pion mass and the large energy required for pion production by photo-nuclear interactions. We discuss this in the next subsection.

The electron path length spectra are nearly extensive in $E_0$ (same for the gamma-ray path lengths). These lie on top of each other when we divide out this initial energy. In
other words, particles in an electromagnetic showers quickly lose information about the initial energy, and such showers are self-similar except for total energy [163]. (This is less true for the hadronic components of the showers.) Consequently, the total path lengths are extensive in $E_0$. Because electron ionization is the dominant dissipative energy-loss process, the total path length of electrons in water is

$$L \simeq \frac{E_0}{2\text{MeV/cm}}.$$  \hspace{1cm} (3.5)

For electromagnetic showers of fixed energy, the total path length for electrons does not fluctuate much. For example, for a 10 GeV electron initiated shower, the average total electron path is $\simeq 5500$ cm, while the standard deviation is only $\simeq 200$ cm. Most of the fluctuations arise from the rare production of hadronic components, for which there is some energy loss without Cherenkov light (e.g., neutrons, nonrelativistic protons). In addition, there is some contribution to the fluctuations because the electron ionization rate depends on energy.

The Cherenkov light intensity is proportional to the electron path length. Figure 3.3 shows that most of the Cherenkov light comes from electrons near the critical energy [162, 163]. The electron path length differences near the endpoints for different injection energies contribute negligibly to the total path length. Also, there is little electron path length accumulated below the Cherenkov threshold. Pion path lengths contribute negligibly because they are much shorter and pions have a higher Cherenkov threshold. In sum, the injection energy of an electromagnetic shower is accurately revealed by its total Cherenkov light. The visible energy of each shower is within a few percent of the true shower energy.

For gamma-ray-initiated showers, the path length spectra of particles (including the hadronic component) are almost identical to those of electron-initiated showers, except near the endpoint, because showers quickly lose information about the initial particle [163].

Spallation isotopes are dominantly produced by particles that produce little (pions) or no (neutrons, gamma rays) Cherenkov light themselves. However, these particles are accompanied by electrons through shower processes. In Sec. 3.3, we detail how to exploit this connection and identify spallation products using Cherenkov light.

### 3.2.2 Hadronic shower spectra

In hadronic interactions in the GeV range and above, the dominant particles produced are pions, with roughly equal numbers of each charge. Hadronic showers of $\pi^-$, $\pi^+$, and $\pi^0$ have much in common with electromagnetic showers of $e^-$, $e^+$, and $\gamma$, because both arise from particle multiplication processes and because the interaction lengths happen to be comparable. Hadronic showers have a critical energy of about 1 GeV, where the probabilities for pions to multiply or to lose energy by ionization are equal. The multiplicity of pions in
Figure 3.4: Electron and pion path length spectra in terms of kinetic energy for showers initiated by charged pions of energy $E_0 = 0.1, 1, 10,$ and $100$ GeV. Again, the features at the endpoints are injection effects. The small features in the electron line for $E_0 = 0.1$ GeV arise due to gamma rays from $\pi^0$ and nuclear decays. All spectra are normalized by $E_0$.

hadronic showers increases with energy, being a few in the GeV range and a few tens in the TeV range [35]. For further discussion, see Refs. [169–173], though note that their focus is on high energies and low densities. In the following, we emphasize some differences between hadronic and electromagnetic showers.

Although electromagnetic showers have, on average, only a small hadronic component, hadronic showers always have a dominant electromagnetic component. Charged pions interact, producing more pions and continuing the hadronic shower. However, neutral pions promptly decay to gamma rays, feeding an electromagnetic shower. With each new generation in the hadronic shower, roughly $1/3$ of the remaining energy is transferred to the electromagnetic shower. In principle, a hadronic shower with enough interactions would transfer all of its energy to the electromagnetic shower; in practice, the final hadronic fraction asymptotes at $\simeq 10\%$ [174, 175]. The number of charged pions reaching low energies is larger than would be naively expected due to large pion multiplicities at high energy and fluctuations in the energy division in each interaction.

Figure 3.4 shows particle path length spectra for showers initiated by charged pions. For $E_0 = 1, 10,$ and $100$ GeV, the primary pions have enough energy to induce hadronic showers; for the $0.1$ GeV case, there is no pion multiplication and we discuss it separately.

The electron and pion spectra are not quite extensive in the injection energy. This can be seen from the fact that the curves shown in Fig. 3.4 do not overlap. With increasing injection energy, the fraction transferred to the electromagnetic shower increases. For $E_0 =$
1, 10, and 100 GeV pion-initiated showers, the fractional energy in electromagnetic showers is 31%, 49%, and 65%. The rest of the energy is dissipated by hadron and muon ionization energy loss, with a small fraction carried away by neutrinos. Accordingly, as the injection energy increases, the pion curves fall and the electron curves rise.

Pion-initiated showers thus appear to be less energetic than electromagnetic showers with the same initial energy. The visible energy is proportional to the total particle path length above the Cherenkov thresholds. The energy that goes into the electromagnetic component of the shower produces Cherenkov light due to the \( \simeq 500 \text{ cm} / \text{GeV} \) of relativistic electron path length. However, the energy that remains in the hadronic component of the shower is less efficient, with only \( \simeq 100-200 \text{ cm} / \text{GeV} \) of relativistic pion path length. The difference is because some energy is lost to neutral particles and because pions become non-relativistic at a higher energy than electrons. In terms of light yield, pions are subdominant even in pion-initiated showers [162]. The visible energies for \( E_0 = 1, 10 \) and 100 GeV pion showers are 0.57, 6.3, and 74 GeV.

The general features of the pion spectrum follow from the same principles that govern the electron spectrum: showering processes dominate at high energies, causing the increase in path length with decreasing energy, while ionization dominates at low energies, causing the decrease in path length with decreasing energy. The critical energy for hadronic showers is higher than that for electromagnetic showers, due to the large pion mass and other factors, and the behavior of the path length spectrum in the peak region is more complex. The peak near 0.4 GeV corresponds the most probable pion production energy. At slightly lower energies, 0.1–0.3 GeV, some pions disappear through inelastic interactions of the form \( \pi^- + p \rightarrow n \) and \( \pi^+ + n \rightarrow p \) with bound nucleons, with the residual energy and momentum absorbed by their nuclei. Once charged pions become nonrelativistic, the ionization rate increases quickly and the path length accumulated is small and decreases more steeply than for electrons below the peak.

When the pion injection energy is too low to create new pions, an electromagnetic shower cannot typically develop. The pion path length spectrum is large, as all the energy remains with the pions, and this is the same for both \( \pi^+ \) and \( \pi^- \). For the \( E_0 = 0.1 \text{ GeV} \) case shown in Fig. 3.4, the total pion path length is 23 cm. Although this curve is much higher than the others, its integral is only slightly larger, corresponding to 230 cm / GeV, because nonrelativistic particles lose energy rapidly. Rarely, a charged pion interacts with a nucleon and converts to a neutral pion, leading to some electromagnetic activity (on average 11 cm of electron path length). Low energy \( \pi^- \) are especially efficient at making isotopes through atomic and then nuclear capture [176]; low energy \( \pi^+ \) do not efficiently make isotopes because they decay, not capture, once at rest.
Figure 3.5: Average longitudinal profiles for showers initiated by electrons of energy $E_0 = 1$, 10 and 100 GeV. Here $dL$ is the charged-particle path length in all directions accumulated in a step $dz = 10 \text{ cm}$ along the initial direction. We separately shift the starting positions of the showers, each with one electron and height $\sim 1/E_0$, so that the peaks line up at $z = 0$. All profiles are normalized by $E_0$.

3.2.3 Shower geometry

The physical distributions of showers and how they compare to the size of the Super-K detector are crucial for understanding why the new Super-K cut technique [26] gives such a big improvement. The longitudinal and lateral sizes of showers define the region around the muon track where isotopes are made. The exact profile and the deflection of shower particles determine the pattern of Cherenkov light. We focus on electromagnetic showers in this section, because they are more common, because hadronic showers have a large electromagnetic shower component, and because hadronic showers are similar to electromagnetic showers in geometry (slightly different, and discussed below).

Figure 3.5 shows the average longitudinal shower profile for three different injection energies. We plot the electron path length per unit length along the initial direction, i.e., the Cherenkov intensity from the shower relative to that from a single particle. This is roughly the instantaneous number of charged particles in the shower times $(\text{GeV}/E_0)$. This is not exactly true due to nonforward motion and particles starting or stopping within bins; in addition, these curves represent averages over many showers. The area under the curve is the total electron path length scaled by the injection energy, and is nearly the same for all energies. The showers extend 4–6 m for energies between 1–100 GeV. This length is much shorter than the height of the Super-K FV, even for high-energy showers, which are rare.

These average profiles show a rising phase, a peak, and a declining phase. The distance
to the peak position of the shower is an important parameter. Even though Eq. (3.2) and Eq. (3.4) were derived from simplified models, they are in good agreement with the full numerical results. In more detail, the shape is consistent with standard formulas for the longitudinal profiles of showers, such as the Greisen [160] and Gaisser-Hillas profiles [177].

The overall profile shape, especially the length asymmetry between the rising and falling parts of the shower, is important for our discussions of shower correlations with spallation backgrounds in Super-K. Compared to the naive Heitler model, where all electrons stop in one radiation length after shower maximum, the tails of realistic showers are long. This arises from two types of fluctuations in showers: the distances particles travel before splitting obey an exponential distribution, and secondary particles do not always split the energy equally [178]. These fluctuations give a distribution to the particle energies in the shower at a given depth, instead of all particles having the same energy at the same location. After

Figure 3.6: Examples of longitudinal profiles (blue bins) for showers initiated by electrons of energy $E_0 = 1, 10$ and $100$ GeV, as well as the averages (thin black lines). All profiles are normalized by $E_0$. 
the shower maximum, there are particles in the shower with energy higher than $E_c$ because they have interacted for fewer generations or because they have taken more energy from their parent particles. These higher-energy particles stay in the shower longer, creating the long tail.

Figure 3.6 shows examples of longitudinal profiles of individual showers, as fluctuations will affect shower reconstruction. Showers with primary energies of 1 GeV look very different from one another and from the average profile. With increasing initial energy, the relative fluctuations in shower profiles decrease. Showers with 100 GeV have little variation in widths, peak position, and shape. Because the shower energy is proportional to the Cherenkov light intensity, it is easy to measure the total energy in a shower (up to the ambiguity of whether it is electromagnetic or hadronic). For high-energy showers, it might be possible to reconstruct them using the average profile as a template. For low-energy showers, which are the most common, it is not clear if template fits will be helpful, due to the large fluctuations.

So far, we have simplified showers to be one dimensional and collinear. Particles in showers do have lateral displacements. The most important reason is electron displacement due to multiple scattering during propagation [159]. This is characterized by the Molière radius, which is about 10 cm in water [35]. This is very small compared to either the Super-K muon track resolution or the distance between the spallation decay and the muon track. The effects of the lateral extent of showers are negligible, so we skip discussions of their average profile or fluctuations.

However, though the lateral displacement of electrons is small on average, their angular deflections greatly affect how the shower appears in the detector. Note from Fig. 3.1 that individual electron paths are short but that deviations away from the forward direction are common. We will discuss this in detail in our next paper.

As noted, hadronic showers are similar to electromagnetic showers in geometry, but there are some differences. For 1 GeV hadronic showers, the longitudinal extent is similar to that shown in Fig. 3.5, but the shape is quite different. Because this is so close to the hadronic critical energy, there are few generations, and we mostly see the average number of pions decrease according to an exponential set by the hadronic interaction length. This might provide a way to identify low-energy hadronic showers, which are especially important for isotope production. The longitudinal profiles for 10 and 100 GeV hadronic showers are quite similar to those of electromagnetic showers. At all energies, the fluctuations in the longitudinal profiles of individual hadronic showers around the average are greater than for electromagnetic shower of the same energy; this might be used to distinguish hadronic showers on a statistical basis. A more promising means might be to use the fact that hadronic showers have larger lateral extent (see Fig. 4 of Ref. [2]).
3.2.4 Shower frequency

Cosmic-ray muons abundantly produce daughter particles that initiate electromagnetic and hadronic showers. Figure 3.7 shows the daughter particle production spectra obtained using the Super-K muon spectrum. The frequencies are scaled by the muon rate in Super-K, and are thus numbers per muon.

The electron spectrum goes as $dN/d\log_{10}E \sim 1/E$. This comes mainly from delta-ray production — collisions of muons with atomic electrons where the energy transfer is large. (Far more frequently, these collisions transfer little energy, and are treated as continuous ionization.) For a muon energy of 270 GeV, the average at Super-K, the maximum energy transfer to an electron is 260 GeV [35]. The differential cross section for delta-ray production scales as $\sim 1/E^2$ for electron energy transfers well below the maximum [35]. This, plus the fact that we plot $dN/d\log_{10}E \sim EdN/dE$, largely explains the results shown.

The positron spectrum comes entirely from pair production, mostly through muon interactions with nuclei. The differential cross section does not have a simple power-law form. Using an approximate formula [128, 179], we find that the differential cross section can be approximated by a broken power law: $\sim E^{-1.5}$ at low energies and $\sim E^{-3}$ at high energies. The transition energy is around $2(m_e/m_\mu)E_\mu$, which is about 2 GeV for the muons in Super-K. Again, reasonable agreement is seen. Electrons are also produced in pair production, and this component is the same as the positron spectrum.

The gamma-ray spectrum is rather flat, which follows from the form of the
bremsstrahlung differential cross section, which is $\sim 1/E$ \cite{35}. Except at the highest energies, showers initiated by gamma rays are subdominant.

The rate of hadronic showers is small because muons primarily lose energy by electromagnetic processes. The dominant hadrons made directly by muons are pions, with comparable numbers of each charge.

Relative to a mono-energetic muon spectrum, using the full Super-K spectrum in Fig. 3.7 (as we do) leads to only modest differences. At the highest energies, the differential cross sections for delta-ray production and pair production quickly increase with muon energy \cite{35}. Consequently, the electron and positron production are increased at high energies. For the other particles and energies, the differences are less.

The spectra of muon daughter particles, and hence the showers they induce, favor low energies. For electromagnetic showers, because of the dominant rate of delta-ray production, the total spectrum has a $dN/d\log_{10}E \sim 1/E$ shape. The delta-ray spectrum does not stop at 0.1 GeV but keeps rising at lower energies. These low-energy delta rays do not shower or make isotopes, but they do create an almost continuous light intensity on top of the flat light profile from the muon, with little variation between muons. The hadronic shower spectrum is relatively flat, with a wide peak near 0.4 GeV. (The hadronic component in electromagnetic showers is of comparable, but smaller frequency.) Though hadronic showers are rare, with rate below 1% of all showers, they are quite important for producing isotopes. To obtain the expected number of all showers per muon above a given energy, we integrate the curves in Fig. 3.7; above 0.1, 1, 10, and 100 GeV, we obtain 3.6, 0.4, 0.04, and 0.003. For each muon, there will be Poisson fluctuations in the number of showers. In Sec. 3.3.2, we calculate the energy distributions of showers weighted by isotope and light production.

### 3.3 Isotopes are born in showers

In our previous paper \cite{2}, we showed that isotopes are typically not produced directly by muons, but rather by their low-energy secondaries. (An exception, discussed in Sec. 3.3.1, is stopping $\mu^-$. ) The isotope yields follow from convolutions of secondary-particle path-length spectra with isotope-production cross sections. Neutrons and pions are the most important secondaries for producing background isotopes — those that decay with detectable signals in Super-K. In contrast, gamma-ray secondaries primarily produce harmless isotopes — those that are stable or decay invisibly. We focus on background isotopes.

In this section, we show that most isotopes are produced in rare, individual showers. On one hand, this is not surprising, because isotope production increases with secondary particle path length, and showers produce many secondaries in a short distance. On the other hand, it has been assumed that isotopes are made continuously along the muon tracks.

A consequence of our claim is that isotopes are produced at random but specific loca-
tions, coincident with showers, along muon tracks. This picture is different from one where we average over muons (as in Ref. [2]), so that isotopes are produced nearly uniformly along the muon track. As we show, showers can identify and localize isotope production, because showers are detectable through their Cherenkov signals.

Using position information for preceding showers, the cuts to reduce spallation decays need to be applied only to a short section of the muon track that effectively covers the shower. Compared to most Super-K analyses, where cuts are made along the whole muon track, this would allow decreased backgrounds without increased deadtime. With the same deadtime, cutting less volume allows a longer time cut, improving background rejection. A version of this technique was pioneered by Super-K in a search for the diffuse supernova neutrino background [26], and it was shown to work to remove spallation backgrounds down to decay energies of 16 MeV. Our goal, besides giving the first explanation of why this technique works, is to show how to extend it down to 6 MeV, where the spallation rate is much higher, and apply it to solar neutrino studies.

In the remainder of this section, we show how light and isotope production correlate with muon energy loss, how they causally depend on the initiating particle and energy of showers, and how well in principle these showers could be identified and localized. We calculate the distributions of products — showers, light, and isotopes — from individual muons. Super-K could use these distributions, following their likelihood approach, to assess the probability that an observed signal is of a particular origin, e.g., if a low-energy event is signal or background (and, if so, which muon was likely the cause).

### 3.3.1 Muon energy loss leads to light and isotopes

There can be several independent showers along a muon track. When that is the case, detecting each shower and measuring its energy would require geometric reconstruction. It is easier to measure the total visible muon energy loss through the total Cherenkov light intensity. The true muon energy loss is slightly larger than the apparent energy loss because of the reduced light yield of hadronic showers.

Increased muon energy loss results in greater path length in secondaries and, hence, more Cherenkov light. Most of the radiative energy loss goes into producing electromagnetic showers, and the subsequent electrons are contained in the detector. Thus Super-K can measure the energy loss (but not the absolute energy) of a throughgoing muon by the total light deposited. The radiative part can be obtained by subtracting the amount expected from a muon with the minimum energy loss (greater than the minimum ionization rate because these muons are relativistic). Even in the rare cases where there are hadronic energy losses, the total light is a reasonably faithful (better than a factor of 2; see above) measurement of the muon energy loss.

Increased muon energy loss results in more isotopes, also due to more secondaries. How-
Figure 3.8: The expected number of background isotopes as a function of the total muon energy loss. The solid line is our calculation assuming vertical throughgoing muons that travel 32.2 m in the FV, and the dashed line is the (corrected to match assumptions) Super-K measurement.

However, there is an important difference: While light production is common, isotope production is rare. Most background isotopes in water are produced by low- to medium-energy hadronic secondaries (see Fig. 7 of Ref. [2]), which are rarely produced and which are subdominant to electromagnetic secondaries. Recall that hadronic showers always induce electromagnetic showers (but not vice versa), and that the light from the latter is typically dominant.

Figure 3.8 shows our calculation of how the production of background isotopes increases with total muon energy loss. We also show the Super-K measurement, which is part of their likelihood function for spallation cuts, defined in terms of residual charge, \( Q_{\text{res}} \), the number of detected photoelectrons in excess of that expected from a muon with the minimum energy loss. We made conversions between residual charge and energy loss for which we could find only an approximate factor \( 1000 \text{ photo-electrons} \simeq 130 \text{ MeV} \) [180]. We assume that the Super-K results are for the expected number of isotopes per muon and that they need to be corrected by a factor \( 1/0.1 \) because only a fraction of isotopes are included by the cuts used to select spallation events; Refs. [14, 96] are not clear about either point. We obtain 0.1 by direct calculation, not \textit{ad hoc} adjustment; this arises from two factors, each \( \simeq 0.3 \), for a time cut of \( \lesssim 0.1 \text{ s} \) and an energy cut of \( \gtrsim 7 \text{ MeV} \). In addition, we assume that all muons are vertically throughgoing. Nevertheless, our estimates should be reasonably accurate. The good agreement with the Super-K measurement indicates that our simulation is correctly modeling muon energy loss and isotope production.

This simple figure illustrates several important points that hint at the physics of isotope
production in showers. First, the average production rate of background isotopes is small, even for large muon energy losses. (The yield of harmless isotopes is about ten times larger.) Second, this function becomes nonzero only beyond about 7 GeV, which is where muon radiative loss processes start [2]. Third, the curve rises faster than linearly for low values of muon energy loss. We separately checked individual isotopes, and found that they follow the same trend as the total shown in the figure.

There are two possible shower frequency scenarios that could lead to Fig. 3.8. A point common to both simply follows from Poisson statistics, which we illustrate using an energy loss of 30 GeV. Because the number of background isotopes per muon is 0.1 on average, the number of isotopes produced is 1 for 1 muon and is 0 for 9 muons. However, Fig. 3.8 does not tell us the frequency of showers that make isotopes. Small electromagnetic showers are more frequent and less efficient at making isotopes. If the isotopes were made by such showers, then the number of showers per muon would be \( \sim 1 \), with a fraction \( \sim 0.1 \) of them making isotopes. Hadronic showers or very energetic electromagnetic showers are less frequent and more efficient at making isotopes. If the isotopes were made in these showers, then the number of such showers per muon would be \( \sim 0.1 \) with a fraction \( \sim 1 \) of them making isotopes. Distinguishing these scenarios is important. If isotope-producing showers were small in energy and common in position, then spallation cuts would have to be applied along the whole muon track; in contrast, if these are big and rare, they could be localized to short regions along the muon track. The physics of isotope production by showers determines which shower energy range is most important.
Although isotope production rises with muon energy loss, the frequency of muon energy loss falls steeply (see Fig. 2 of Ref. [2]). When the muon energy loss is large, strong cuts can be applied without increasing deadtime because the frequency of such events is low. For example, *muon energy losses of 30 GeV or more lead to $\simeq 60\%$ of the isotopes in Super-K, while being only 2% of all muons.* A simple cylinder cut along the muon track could thus eliminate a majority of isotopes with little deadtime. Using a radius of 3 m and delay of 20 s for just the muons with large energy losses, Super-K could cut $\simeq 58\%$ of isotopes with only $\simeq 4\%$ deadtime. (For comparison, a radius of 1 m and a delay of 20 s, applied to all muons, would cut $\simeq 80\%$ of isotopes with $\simeq 20\%$ deadtime, close to what Super-K achieves with more sophisticated likelihood techniques.) In Ref. [26], Super-K introduced a new cut on “showering muons,” defined to be those with an energy loss $\gtrsim 60$ GeV; for these, all data in the next 4 s from the whole detector are discarded. We estimate that this has substantially worse efficiency and deadtime than our proposed new cut.

Our investigations also demonstrate that no spallation cuts are necessary along the tracks of stopping muons. Muons with low energy ($\lesssim 7$ GeV) lose all their energy by ionization in the FV. Because their energies are low, they do not typically lose energy by radiative processes. Consequently, very few isotopes (0.4% of all isotopes) are produced along their tracks. At the ends of their tracks, however, negative muons can capture on oxygen, which can lead to nuclear breakup. Thus, a separate cut for stopping muons where only events inside a sphere centered on the end of the muon track are rejected would be highly efficient with minimal deadtime (Super-K has such a cut for $^{16}$N [23]).

Figure 3.10 shows our results for the average yields of light and isotopes made by showers as a function of energy. The shape of the histogram is the frequency of muon energy loss in Super-K (Fig. 2 of Ref. [2]) multiplied with the yield of isotopes from muons in Super-K (Fig. 3.8). We focus on a small energy range (below 30 GeV), assuming that high-energy-loss muons can be cut as suggested above. This figure shows that the most probable energy loss for isotope production is small. However, there is a long tail, extending to hundreds of GeV. Once the energy loss range is constrained to a reasonable range, the cut should be optimized for small energy losses.

### 3.3.2 Individual showers are the cause

When we average over muons and along their tracks, as above, light and isotope production are correlated through the total muon energy loss. Here we break that energy loss into individual showers, and detail how light and isotopes are causally related to showers with different injection energies and initiating particles. These relationships determine the geometry of the spallation cuts.

Figure 3.10 shows our results for the average yields of light and isotopes made by showers as a function of energy. To calculate how muon-induced showers produce light and
isotopes, we obtain the number spectra of daughter particles produced directly by muons using Fig. 3.7, then multiply these number spectra with the yields of light and isotopes by showers with those energies. This approach accounts for nearly all the daughter particles from the radiative energy losses of muons; we discuss the exceptions below. We define showers initiated by $\pi^\pm$ (including a small contribution from kaons and other hadrons) to be hadronic, and those initiated by $e^\pm$, $\gamma$, or $\pi^0$ to be electromagnetic. To compare to experiment, we use visible energy, determined from the total Cherenkov light (proportional to the integrated path length above the Cherenkov thresholds) made by relativistic particles (see Sec. 3.2.1, 3.2.2). At injection energies below 0.1 GeV, the curves drop off because showers do not form; at energies above $10^3$ GeV, they drop off because such injection energies are rare.

An immediate conclusion is that light production is strongly dominated by electromagnetic showers, which are by far the most common. Another is that background isotope production is somewhat dominated by hadronic showers, even though they are much more rare.

The light yield distributions depend on the physics of muon energy loss and of shower development. At lowest order, the light yield $dL/d\log_{10} E$ follows $E dN/d\log_{10} E$, which can be obtained by multiplying Fig. 3.7 by $E$. Electromagnetic showers in this energy range are primarily induced by delta rays from muons, and their frequency falls as $\simeq 1$ (GeV/$E_0$)
shower per energy decade per muon traveling the length of the Super-K FV (3220 cm). The light yield of an electromagnetic shower rises as $\simeq 500 \text{ cm} \left( E_0 / \text{GeV} \right)$. In combination, the result is $\simeq 500 \text{ cm}$, almost independent of shower energy. (This continues to even lower energies, dropping slightly, due to low-energy delta rays.) That is, 5000 cm of light is equally likely to be from one 10 GeV shower or ten 1 GeV showers; these cases can be distinguished by reconstruction of the light profile along the muon track. Hadronic showers in this energy range are primarily induced by pions from muons; the rate relative to delta-ray production is $\sim 10^{-2}$ near 1 GeV but increases steeply with injection energy. Hadronic showers convert most of their energy to electromagnetic showers, which produce nearly all of the light, and this efficiency increases with injection energy. The light yield for hadronic showers as a class is therefore quite suppressed and is not as flat as for electromagnetic showers. At low energies, this variation is especially pronounced because of low pion production by muons. The total light yields (integrated over energy) provide an important check of our calculation. The average light yield per muon is $\simeq 2000 \text{ cm}$, corresponding to a radiative energy loss of about 4 GeV, or a total energy loss of about 11 GeV, in good agreement with the average we found in Ref. [2].

The isotope yield distributions depend on similar physics, plus the interaction cross sections of secondaries with nuclei. Although the frequency of hadronic showers is low, the neutrons and pions they produce are quite efficient at making background isotopes. (Above a total muon energy loss of about 30 GeV, this efficiency is so high that it becomes possible that 2 or more isotopes are produced in the same shower, which would allow their clear identification and localization as background events.) EM showers make isotopes mostly through the neutrons and pions they produce, but also directly through gamma rays. The shapes of the isotope distributions are similar to each other and to the light distributions, but there are some important differences. Low-energy hadronic showers are especially efficient (per injected energy) at making isotopes, because they convert less of their energy to electromagnetic showers; low-energy electromagnetic showers are especially inefficient because of the threshold energy needed to induce hadronic showers. The shape of the isotope production curve here is closely related to that in Fig. 3.9. Here we consider the energy of individual showers, each of which contributes to the radiative energy loss; the total energy loss in Fig. 3.9 includes about 7 GeV for ionization energy loss. Also, here we use a log axis, which stretches out small radiative losses, and a log derivative, which has the effect of multiplying the shape by a factor $\sim E$.

These facts show why the total muon energy loss and isotope production are correlated but not causally connected. Most of the detected muon energy loss comes from electromagnetic showers. In contrast, most isotopes are made by hadronic showers. Both types of shower increase with muon energy loss. The correlation between energy loss and isotope production is not simply linear because of the steep rise of isotope production as a function
of shower energy at low energies. Even at the level of individual showers, the production of light and isotope production are not completely causal. The isotope production per shower is typically low, which means the presence of a shower does not necessarily indicate the production of an isotope. However, when an isotope is produced, it is almost always preceded by light from a shower, and that is what makes the Super-K background-reduction technique possible.

How well the Super-K technique works depends on the frequency of showers that make isotopes. *The drop in isotope production in low energy showers shown in Fig. 3.10 is crucial.* Few isotopes are made by low-energy showers, which are common, or low-energy delta rays, which are near continuous. From Fig. 3.7, we calculate that the integrated rate of showers becomes \( \simeq 1 \) per muon when the minimum daughter particle energy is \( \simeq 0.4 \) GeV. Because almost all isotopes are made by higher-energy showers, this technique can work with minimal confusion about which shower to associate with an isotope. If low-energy showers had produced too large a fraction of isotopes, the associated showers would be too frequent along the muon track for this technique to be practical.

How well the Super-K technique works also depends on the fraction of background isotopes produced in showers. Figure 3.11 shows the fraction of isotopes contained in showers above a given energy. The curves are integrations of the isotope yield curves in Fig. 3.10, now using true shower energy. The hadronic and electromagnetic components
shown in Fig. 3.11 are the same as in Fig. 3.10. The neutron component, not shown in Fig. 3.10 because it produces so little light, is special. Above a few hundred MeV, neutron secondaries act as part of the hadronic component. At lower energies, they can induce “neutronic” showers, where neutrons collide with nuclei, ejecting neutrons (and protons), continuing the process, producing isotopes but very little light; this accounts for only a few percent of isotopes.

Figure 3.11 shows that nearly all isotopes are made in showers induced by muon daughter particles, which is also crucial for this technique. (We exclude isotopes made directly by primary muons, which make 3% of all isotopes, mostly through processes that then produce identifiable showers.) Above 0.01 GeV, we recover 96% of the isotopes that are not directly produced by primary muons. Within the precision of our calculations, this agrees well with the isotope yield in Ref. [2], where we did not separate the processes leading to isotope production. This supports our claim that nearly all isotopes are made in showers. In future work, we will show that nearly all of the showers in Fig. 3.11 are identifiable.

3.3.3 Showers can tag isotope production

The results above show that isotopes are almost always produced in showers, and that these showers are detectable by their light. The probability of isotope production increases with shower energy, though it is small at the most important energies. These facts agree with the usual Super-K spallation likelihood function, for which isotope production increases with the total muon energy loss. If this energy loss can be localized to a shower, it will allow the cut to be applied to a shorter section of muon track. The success of the Super-K cut technique depends on the fraction of isotopes produced in identifiable showers.

Figure 3.12 shows the distribution of separation distances between the peak of the muon light profile and isotope production point. We first describe our calculation in detail, and then compare to the Super-K result. For each individual muon, the peak of the muon light profile is taken to be the point of the maximum charged particle path length along this muon track. We define the $z$ coordinate to increase along the muon track, beginning at the top of the detector, and the separation distance to be the $z$ position of the shower minus that of the isotope. For calculating the maximum light position, we use a binning of 50 cm, comparable to the position resolution in Super-K at low energies; other reasonable choices give similar results. When more than one isotope is produced, we compute the separation distances for each. Because of how the distribution is defined and would be used in a likelihood approach, there is no conceptual problem with having more than one isotope produced by one muon. Practically speaking, the most common such scenario should be two isotopes produced in a rare, high-energy shower.

The separation distribution has a large peak and small tails. The peak comes from the case where the isotope is produced in the largest shower along the muon track. The isotope
Figure 3.12: The longitudinal separation distribution between showers and isotopes. The solid line is our calculation assuming a perfect shower reconstruction technique, and the dashed line is the Super-K measurement. The Super-K technique already works very well but could be significantly improved.

production profile generally follows the shower longitudinal profile. The peak in Fig. 3.12 is thus centered at zero. The full width of the peak of $\sim 4$ m at half-maximum follows from that of the longitudinal shower profiles; it extends further to the left because showers are longer after the peak than before. Because the peak is quite sharp, it can define a new spallation likelihood function with stronger cuts over a shorter section of muon track, as empirically discovered in Ref. [26]. The tails, which can be barely seen at separations of tens of meters, arise from cases where the isotopes and showers are uncorrelated. As the distributions of showers and isotopes are nearly flat along the muon track, the tails have a well-defined shape — a symmetric triangle peaked at zero separation. For our calculation, we find that the area in this triangle is 13% of the total.

To improve background rejection, it is important to understand the reasons for this uncorrelated component. We find that $\sim 3\%$ is due to isotope production accompanied by very little light; the parent particles are high-energy muons or low-energy neutrons made by them, in a ratio of about 1 to 2. The largest portion, $\sim 10\%$, is due to cases where the isotope is produced in a visible shower, but where there is a larger shower elsewhere on the muon track; we determine this by examining isotope-shower pairs with large separations. As a check, we find that this portion increases if we increase the height of the simulated detector. A key issue for reducing the uncorrelated component will thus be improving the identification of multiple independent showers along the muon track. The uncorrelated component is as small as it is, even with this simple approach, because the expected number
of showers per muon is small.

Figure 3.12 also shows the Super-K result from Ref. [26]. Although it is similar, there are some important differences. The most important is that the area in the tails is \( \simeq 25\% \) instead of 13\%. This excess is due to cases where the isotope is produced in a shower that would have been visible in our simulation but was not visible in the Super-K analysis, at least after the smearing effects of imperfect Cherenkov reconstruction. We can approximately recover the Super-K fraction of \( \simeq 25\% \) if we assume that showers below \( \simeq 10 \text{ GeV} \) (muon energy losses below \( \simeq 17 \text{ GeV} \)) cannot be reconstructed. In addition, the peak and tails are not symmetric, which we think is due to problems with shower reconstruction, as discussed in our next paper. Our estimates about the Super-K results are crude, as their analysis has low statistics and large bin widths (this could be improved by their using spallation decay energies lower than 16 MeV); the functions used to fit their data seem nonideal; the noted asymmetries cause uncertainties; and there is the possibility of differences in the selection of single-throughgoing muons in the Super-K analysis and in our simulations.

There are two major steps Super-K can take to strengthen the correlation between showers and isotopes. First, they could attempt to reconstruct showers of lower energy. A \( \sim 10 \text{ GeV} \) shower more than doubles the light from a muon track, and we expect that much smaller showers could be identified. If they can do this down to very low energies, their measured result should match what we obtained in our simulated data, and they could reduce \( \simeq 25\% \) to \( \simeq 13\% \). Second, they could attempt to recognize multiple showers per muon, defining cut regions around each. Because showers are relatively rare, it would probably be enough to reconstruct up to two showers. If this were successful, they could reduce \( \simeq 13\% \) down to \( \simeq 3\% \).

In future work, we will show that it should be possible for Super-K to improve their reconstruction technique well enough to match our results in Fig. 3.12, and then even further, i.e., reducing the tails of the distribution function with new methods. This will allow significantly better background rejection.

### 3.4 Conclusions and Future Work

Low-energy neutrino detectors could continue to provide invaluable information about the Sun, supernovae, and neutrino properties. Prominent goals include the \textit{hep} solar flux, the DSNB flux, and the solar day-night mixing effect. Super-K is large enough, but progress depends on reducing detector backgrounds. In the energy range 6–18 MeV, the dominant background is from the beta decays of unstable nuclei produced by cosmic-ray muons and their secondaries. Super-K has strong cuts to reduce these backgrounds, but the residual rates are large.

We are undertaking a multipart project to provide tools to significantly reduce these
spallation backgrounds in Super-K. Our project, based on a foundation of careful simulation and theoretical insights, is the most extensive such effort undertaken for any detector. With modest adjustments, our results will be useful for other water-based detectors, e.g., WATCHMAN [181] and Hyper-Kamiokande [142]. Since these detectors are likely to be shallower than Super-K, spallation backgrounds will be even more severe. More generally, our results will provide valuable insights about backgrounds in other underground detectors for neutrinos, dark matter, and other rare processes such as neutrinoless double beta decay.

In our previous paper [2], we presented the first theoretical calculation of the spallation background yields in Super-K. We focused on the steady-state background rates, averaged over muons and along their tracks. We found that almost all isotopes are produced by secondary particles, and not the primary muons themselves. Our predictions for the spallation decay backgrounds agree with Super-K aggregate data to within a factor of 2, which is very good and could be improved. Our results provide new information about components, correlations, and production mechanisms that can be used to develop cuts that are more powerful than those based on empirical studies.

Our next steps were inspired by a recent Super-K DSNB analysis [26], where the Cherenkov light profiles associated with individual muons were measured. These were found to vary along the muon tracks, showing peaks, with the positions of the peaks correlated with the sites of isotope production. A new cut was developed using this correlation, and was shown to be effective for improving the DSNB search. However, the cause for the variation in the light profile and its correlation with isotope production remained mysteries. This new cut has not yet been used for solar neutrino analysis. It seems very promising for reducing backgrounds without increasing deadtime.

In the present paper, we consider how isotope production varies between muons and along their tracks. We break the process of muons producing isotopes into muons producing energetic daughter particles, these daughter particles inducing electromagnetic and hadronic showers, and these showers producing isotopes. We provide details about each step and combine them in the end. Our calculations here break our previous calculations [2] into more steps, but agree in overall approach and results.

Our fundamental result is that showers are the key to explaining the correlation between muon light profiles and spallation backgrounds, as well as their total yields of spallation products in Super-K. Showers produce electrons, which make Cherenkov light, and neutrons and pions, which make background isotopes. In Fig. 3.10, we show how showers of different types and energies contribute to the production of light and isotopes. Because of the high rate of electromagnetic showers, and the high efficiency of hadronic showers for making isotopes, electromagnetic showers strongly dominate light production and hadronic showers somewhat dominate isotope production. Isotopes are nearly always proceeded by showers, though only a small fraction of showers produce isotopes. With these results, we reproduce
Super-K results on muon energy loss (Fig. 3.8), isotope production (Fig. 3.11), and their correlations (Fig. 3.12).

We are the first to show that the background isotopes in Super-K are dominantly made in discrete, identifiable showers. (It has long been known that isotope production is associated with muons with high radiative energy loss, e.g., Refs. [182, 183] and much subsequent work, but it had not been shown that these showers are rare enough and energetic enough to be identifiable, and that they account for the production of nearly all isotopes.) Though this paper focuses on Super-K, our results have much more general applicability.

The calculations and insights of this paper and of Ref. [2] can be used to define new cuts that should be very effective for solar and DSNB analyses. Some could be implemented easily (the muon energy loss and stopping muon cuts in Sec. 3.3.1); others improve the technique of Ref. [26] (the efficiency of the technique depends on how well Super-K reconstructs the muon light profile, Sec. 3.3.3); and others need new development (our forthcoming papers).

We will soon demonstrate new ways to better identify showers. As mentioned above, the Super-K reconstructed light profiles are inconsistent with what we expect from showers. In our next paper, we identify the reason for this inconsistency and will demonstrate better ways to reconstruct muon Cherenkov light profiles. In the Super-K reconstruction equation, which solves for the emission position of each individual photomultiplier hit, there are two possible solutions for the light from deflected electrons; we will show how to select the better solution, and that doing so improves the resolution. In addition, we will show how to isolate shower light from muon light, which also helps significantly. In subsequent papers, we will discuss new signals that can identify showers with even higher efficiency, followed by quantitative studies of the effects of new cuts on background rates and the implications for solar and supernova neutrino analyses.

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Chapter 4

Tagging Spallation Backgrounds with Showers in Water Cherenkov Detectors

Cosmic-ray muons and especially their secondaries break apart nuclei (“spallation”) and produce fast neutrons and beta-decay isotopes, which are backgrounds for low-energy experiments. In Super-Kamiokande, these beta decays are the dominant background in 6–18 MeV, relevant for solar neutrinos and the diffuse supernova neutrino background. In a previous paper, we showed that these spallation isotopes are produced primarily in showers, instead of in isolation. This explains an empirical spatial correlation between a peak in the muon Cherenkov light profile and the spallation decay, which Super-Kamiokande used to develop a new spallation cut. However, the muon light profiles that Super-Kamiokande measured are grossly inconsistent with shower physics. We show how to resolve this discrepancy and how to reconstruct accurate profiles of muons and their showers from their Cherenkov light. We propose a new spallation cut based on these improved profiles and quantify its effects. Our results can significantly benefit low-energy studies in Super-Kamiokande, and will be especially important for detectors at shallower depths, like the proposed Hyper-Kamiokande.

The contents of this chapter were published in Ref. [4].

4.1 Introduction

Astrophysical neutrinos can reveal the extreme physical conditions in their sources as well as new information about neutrino properties. In the MeV energy range, the key targets are solar neutrinos and the diffuse supernova neutrino background (DSNB). Solar neutrinos have been detected for half a century, yet there are still unanswered questions [24, 100, 105, 141, 143, 145]. The upper limit on the DSNB flux is within a factor of a few of theoretical predictions [26, 93, 94, 146–148, 150].

Super-Kamiokande (Super-K) is a 50-kton water Cherenkov neutrino detector [87, 88].
Due to its large volume, low backgrounds, and long running time, Super-K has the best sensitivity to the high-energy, low-flux branches of the solar neutrinos and to the DSNB.

In Super-K, these measurements are background limited. The dominant background in 6–18 MeV is the spallation background [14, 24, 25, 90], which consists of beta decays from unstable isotopes produced by muons and especially their secondary particles [2]. These backgrounds are reduced by associating them with their muon parents, which can be difficult because some of these isotopes have long lifetimes (several seconds) compared to the muon rate (∼2 Hz) [14].

In our first paper in this series [2], the only theoretical study of spallation in water, we calculated the average spallation yields in Super-K. We compared the aggregate time profile and energy spectrum of spallation decays to Super-K measurements, finding agreement within uncertainties. We showed that almost all isotopes are made by secondary particles, e.g., neutrons, pions, and gamma rays, instead of primary muons.

In our second paper [3], we showed for the first time that almost all spallation isotopes are made in muon-induced showers. These showers have high densities of secondary particles; they extend only ∼5 m along muon tracks, while the height of the Super-K detector is ∼40 m. Because showers can be detected through their Cherenkov light, this provides a new way to identify where a spallation isotope might be produced along the muon track.

Earlier, Super-K empirically found variations in the Cherenkov light intensity along muon tracks, and a correlation between the position of the peak and the spallation decay [26]. They developed a new spallation cut based on the measured correlation. Using this, they lowered the analysis energy threshold for the DSNB search. However, the physical cause of the light variations and their correlation with spallation were unexplained. Also, they did not apply this cut to their solar neutrino analysis.

Our finding that most spallation isotopes are made in showers explains Super-K observations, except one. Their reconstructed muon light profiles are much broader and have much smaller amplitude than those expected from showers. Here we show how this discrepancy can be explained by shortcomings of the Super-K reconstruction method, and how to improve it. We explore applications of better-reconstructed profiles. Our results should greatly benefit their solar neutrino and DSNB analyses. Although we use Super-K as an example and attempt to model its main present features, our focus is more general.

For our calculations, we use the simulation package FLUKA (version 2011.2c.0) [84, 85]. It incorporates all the relevant physics for muon interactions in water. Our physics choices for FLUKA are the same as in our previous papers [2, 3]. We simulate throughgoing muons vertically down the center of the Super-K detector; our results can be applied to more general cases. The muon spectrum is shown in Fig. 1 of Ref. [2]. At the Super-K depth (2700 meter water equivalent), the average muon energy is 270 GeV [2, 22].

One difference in our setup here is that our simulation region is the whole Super-K inner
detector (ID), whereas in our previous papers we used only the fiducial volume. The ID is a cylinder 33.8 m in diameter and 36.2 m in height [87]. It is separated from the outer detector by opaque walls (including ceiling and floor), where photomultiplier tubes (PMTs) are mounted [87]. The fiducial volume is an analysis region inside and smaller than the ID (22.5 kton versus 32 kton) [87]. The PMTs collect light emitted in the whole ID, so we use it for our simulation volume.

This paper is organized as follows. In Sec. 4.2, we discuss the basics of shower physics and muon light profiles. In Sec. 4.3, we review the Super-K reconstruction method and how to improve it. In Sec. 4.4, we explore further applications of better-reconstructed shower profiles and quantify how much they could improve the spallation cut. We conclude in Sec. 4.5.

### 4.2 Muon Cherenkov Light Profiles

Relativistic charged particles in water emit Cherenkov light along their paths. The Cherenkov photons propagate through the detector, occasionally getting scattered or absorbed. Some of the photons reach PMTs and are detected. The light intensity (number of photons per distance) emitted by a singly charged particle per unit distance is constant, independent of the particle type and energy [155]. The total number of photons is proportional to the energy deposited, and their arrival positions and times carry information about the event geometry.

When cosmic-ray muons pass through Super-K, they produce charged secondary particles, such as electrons and pions. (With these generic terms, we typically mean $e^\pm$ and $\pi^\pm$; we separate $\pi^0$.) The production and energy loss of secondary particles is prompt, much faster than muons crossing the Super-K ID ($\sim 100$ ns). It is thus not straightforward to separate the Cherenkov light from cosmic-ray muons and their secondaries.

We call the Cherenkov light intensity along a muon track the muon light profile. Its fluctuations reveal secondary production, because the light intensity from muons is constant. To better describe the production of secondaries, we separate it into two steps: a primary muon directly produces daughter particles, and these daughter particles subsequently produce other secondary particles.

We quantify charged particles not by their number, but by the distance they travel, which is proportional to their Cherenkov light emission. In FLUKA, charged particles are propagated by track segments. The Cherenkov light emission from each segment is proportional to its length.
4.2.1 Muon-produced Charged Particles

The energy loss rate of a muon is

\[-\langle \frac{dE_\mu}{dx} \rangle = \alpha + \beta E_\mu, \]

(4.1)

where the brackets indicate averaging over distance [35]. The \( \alpha \) term is for ionization loss, and the \( \beta E_\mu \) term is for radiative loss. At the Super-K depth, where \( \langle E_\mu \rangle = 270 \text{ GeV} \), \( \alpha \simeq 2.9 \text{ MeV cm}^{-1} \) and \( \beta \langle E_\mu \rangle \simeq 0.7 \text{ MeV cm}^{-1} \) [35, 127].

Ionization is muons losing energy by scattering bound electrons [35]. We can further divide this term based on the energy of the outgoing electrons. When their energy is small, this is restricted ionization; when it is large, this is delta-ray production [35]. Restricted ionization loss is a continuous process, while delta-ray production is discrete interactions. The boundary between these two cases is somewhat arbitrary [85]; we set it to be the electron Cherenkov threshold (kinetic energy 0.257 MeV). The average total ionization energy loss for a muon that travels vertically through the ID is \( \simeq 10 \text{ GeV} \), with \( \simeq 6 \text{ GeV} \) due to the restricted loss and \( \simeq 4 \text{ GeV} \) due to delta-ray production [2].

Radiative processes include pair-production, bremsstrahlung, and photonuclear interactions [35]. These are muons interacting with nuclei and producing electron-positron pairs, gamma rays, pions, and other mesons. All of these processes have a large energy transfer for each discrete interaction (up to hundreds of GeV [35]), and the interaction rates are low. The total radiative energy loss through the ID is \( \simeq 3 \text{ GeV} \). All the energy that goes into radiative processes is carried by secondary particles, and mostly dissipates through ionization of these secondary particles. Because of this, there is a near-constant relationship between energy loss and Cherenkov yield. For the production spectra of daughter particles by muons in Super-K, see Fig. 7 of Ref. [3].

The fluctuation levels of the energy losses determine the features of muon light profiles. The restricted ionization loss has negligible fluctuations along muon tracks, and among different muons. The delta-ray production and radiative energy losses have large fluctuations. Even though, on average, these terms are smaller than the restricted ionization, they can be much larger for individual muons. We show how these features affect muon light profiles in the next subsection.

The energetic daughter particles from delta-ray production and radiative processes produce many secondary particles by inducing electromagnetic and hadronic showers [3]. A shower is a series of repetitive interactions where particles interact and multiply in number and decrease in energy. When the average particle energy in the shower is too low to create new particles, particles range out by ionization. An electromagnetic shower is mostly gamma rays producing electrons and positrons by pair production, and electrons and positrons producing gamma rays by bremsstrahlung. A hadronic shower is mostly
charged pions producing multiple charged and neutral pions, and neutral pions decaying to gamma rays and inducing electromagnetic showers.

An important energy scale for showers is the critical energy \( E_c \); showers develop when the average particle energy is above it, and die out below it. In water, \( E_c \approx 100 \text{ MeV} \) for electromagnetic showers [35] and \( E_c \approx 1 \text{ GeV} \) for hadronic showers [3]. Most showers in Super-K have energies \( \approx 1–300 \text{ GeV} \) [3].

Because most shower particles are energetic and have small deflections, showers look like long thin cylinders in real space (an example is shown in Fig. 1 of Ref. [3]). In terms of Cherenkov light production, the dominant contribution for either kind of shower comes from electrons near \( E_c \approx 100 \text{ MeV} \). The average deflection of electrons is \( \langle \cos \theta_z \rangle \approx 0.8 \). Showers in Super-K extend \( \approx 5 \text{ m} \) in the longitudinal direction, and \( \approx 10 \text{ cm} \) in the lateral direction (in hadronic showers, this can be \( \approx 1 \text{ m} \)) [3]. For a detailed discussion of shower geometry in Super-K, see Sec. IIIC of Ref. [3].

Muon daughter particles with energy below \( E_c \) do not induce showers. The most common such particles are electrons. Even though these electrons do not induce showers, they are important for our discussions because they emit Cherenkov light. We refer to them as low-energy delta rays, i.e., electrons with energy above their Cherenkov threshold but below about 100 MeV. We include in this a \( \approx 5\% \) contribution of low-energy electrons plus positrons from pair production.

Shower physics is the key to understanding how to use Cherenkov light to tag spallation backgrounds. There are abundant electrons in electromagnetic and hadronic showers, so
showers can be observed through their Cherenkov light. There are few (many) pions and neutrons in electromagnetic (hadronic) showers, and they efficiently make isotopes. By observing the light from a shower, Super-K could identify its position and thus the position where spallation decays might occur [3]. However, the light profiles observed by Super-K [26, 151] look very different from what we expect from showers. We take a closer look at this next.

4.2.2 Real vs. Reconstructed Muon Light Profiles

To utilize the correlation between showers and spallation decays, we need to know what showers look like in the detector. In this subsection, we first study real muon light profiles, focusing on the shower shape. By real we mean what reconstructed profiles would look like if every detected photon were reconstructed to its correct emission position; the profiles are simulated. We then look at the differences between these profiles and those reconstructed from Super-K data.

Figure 4.1 shows an example of a real muon light profile. We simulate a vertical through-going muon in the ID and plot the total path length of relativistic charged particles relative to the muon path length. This is equivalent to the Cherenkov light intensity in units of that from a single muon. We adopt this unit because it is not affected by experimental effects, such as photon absorption and detector efficiency. For this and similar figures, we use a bin size of 0.5 m, to be consistent with Super-K [26].
The area under the curve is proportional to the muon energy loss. A height of 1 corresponds to only restricted muon ionization energy loss. Any height larger than 1 is due to ionization of additional charged particles, which are produced through delta-ray production or radiative processes.

Though just a single example, Fig. 4.1 is representative. When muons are not showering, their profiles all look similar, with the relative intensity fluctuating between 1 and 2 due to the muon plus low-energy delta rays (the height is sometimes < 1 due to binning issues). The average level is about 1.3, which corresponds to an extra energy loss of 0.5 MeV cm\(^{-1}\) due to low-energy delta rays. The muon profile in Fig. 4.1 shows one energetic shower of energy \(\simeq 15\) GeV. (This example peaks near the center of the detector; showers can occur anywhere along the muon track.) It is quite typical, extending \(\sim 5\) m along the muon track and with a height of about 30. For a shower of energy \(E_0\), the peak height is typically 2–3 \((E_0/\text{GeV})\) [3].

The distance between the peak position of the light profile and a candidate signal event is used to determine the probability of the event being a spallation decay [26]. In other words, Super-K keeps the peak position and discards information about the shape of the muon light profile. In Sec. 4.4, we discuss how this can be improved.

The number of showers and the shower energies vary a lot for each muon [3]. The more energetic the daughter particle, the more rare it is. Low-energy showers are thus more common than high-energy showers. The average number of showers above 1 GeV per vertically throughgoing muon in Super-K is 0.4. It is most common to have zero or one shower per muon. Multiple showers along one muon track happen less than 10% of the time.

Super-K measured the variations of muon light intensity in Ref. [26]. Though their approach is fairly general, it is not based on showers, in which electron deflections play a crucial role. In the next section, we discuss how this affects muon light profile reconstruction.

Figure 4.2 shows an example of a reconstructed muon profile from Super-K (another is Fig. 4.2 of Ref. [151]). Their original y axis is in units of number of photoelectrons detected. We convert that to our units by using 7 p.e. \(\simeq 1\) MeV [184], which includes Cherenkov photon yield, photon absorption, and detector efficiency, etc. This relation is not exact, but it does not affect our discussions.

This light profile varies along the entire muon track, showing a prominent peak in the middle. The full width of the peak is about 20 m and its height is about 10. We estimate that the excess light corresponds to about 15 GeV, similar to the example shown in Fig. 4.1. Beyond 32 m, the falloff in intensity is probably because this muon track left the ID.

It is puzzling why the reconstructed profile looks like this. Even though the shower in Fig. 4.1 is only one realization, it is representative of a shower of a similar energy. The success of the current Super-K cut indicates that their average reconstructed peak position,
at least for large muon energy losses, is quite robust. In the next section, we explain the differences in the muon light profiles, and how to improve the Super-K reconstruction method to get accurate light profiles.

4.3 Shower Reconstruction

It is important to understand the discrepancy between the real and reconstructed muon light profiles. First, it is crucial to the proof that showers are the true cause of the variation in muon light intensity and that spallation isotopes are made in showers. Second, as we pointed out in Ref. [3], the correlation function Super-K measured is not as sharp as the one we calculated using real shower profiles. If Super-K could better reconstruct every shower, even if its energy is low or if it is accompanied by other showers, it would improve the efficiency of the spallation cut.

It is difficult to reconstruct the muon light profile. During a shower, there are many charged particles emitting light at nearly the same time and position, but pointing in different directions, so it would be very difficult to resolve individual rings in the pattern of PMT hits on the wall. Furthermore, the light from showers at specific locations must be separated from the continuous light from the muon itself and from low-energy delta rays.

In this section, we use our knowledge of showers, which are not mentioned in the Super-K paper, to examine the Super-K reconstruction method and its results. We start by reviewing the setup of the equation that Super-K used for reconstruction. Then we study in detail its properties and how its solutions are affected by physical and detector limitations. We present ways to improve their method, demonstrating that we can reconstruct the muon light profile with high fidelity, including identifying showers and measuring their energy, position, and extent.

We first assume that the times of individual detected photons at a given PMT can be measured separately. Then, in Sec. 4.3.4, we discuss complications to that in Super-K and possible solutions.

4.3.1 Super-K Reconstruction Method

To reconstruct a muon light profile, Super-K performed backward fitting using individual PMT hits, without consideration of their correlations. For each PMT hit (taken here to be one detected photon), they measured its position and time and solved for where along the muon track the photon was emitted. They repeated this for all hits from one muon, and got the number of detected photons as a function of the emission position along the muon track, i.e., the muon light profile.

There is no confusion about which muon to associate a photon with, because photons from one muon arrive at the walls within $\sim 100$ ns, and the average time between muons is
Figure 4.3: Diagram for reconstruction of the muon Cherenkov light profile. A photon is emitted from the muon track $\hat{\mu}$ at time $t_e$ and distance $x_1$, propagates a distance $x_2$, and hits a PMT at time $t$ and position $\vec{r}$. The blue triangle (with corners marked by $t_0, t_e, t$) is described by Eq. (4.2) and the green curve by Eq. (4.3); they cross at the solutions of Eq. (4.4), of which only one is marked.

$\sim 0.5$ s (muon bundles are treated separately). In addition, the short duration of the signal means that photons from unrelated low-energy decay backgrounds can be ignored. Finally, because the water is so clear, the effects of light absorption and scattering are minimal.

Figure 4.3 illustrates the geometry. A muon enters the ID at time $t_0$ and moves along the direction $\hat{\mu}$ with speed $c$. A Cherenkov photon is emitted at time $t_e$, a distance $x_1 = c(t_e - t_0)$ along the muon track by either the primary muon or a secondary charged particle. The photon propagates a distance $x_2$ to the PMT with group velocity $c/n_g$ [185–187] ($n_g = 1.38$ for water). The photon hits the PMT at time $t$, where its position is $\vec{r}$ relative to the muon entry point. Because this method treats one detected photon at a time, in essence redrawing Fig. 4.3 for each one, it is easy to accommodate muons at arbitrary positions and angles, as well as PMT hits on the ceiling or floor of the ID. The azimuthal angle of each PMT hit in fixed detector coordinate is needed to define the plane of Fig. 4.3, after which it is not used.

In Fig. 4.3, the muon position at every instant, and thus $\hat{\mu}$ and $t_0$, is known because the entry and exit points and times are determined using inner and outer detector information. The PMT hit time $t$ and its position relative to the beginning of the muon track, $\vec{r}$, are measured. The angle $\theta$ is known immediately.

The angle $\alpha$ can be obtained after solving for $x_1$ and $t_e$. For photons emitted by primary muons, $\alpha$ is the Cherenkov angle $\alpha_0$, defined by the photon phase velocity via
\[
\cos \alpha_0 = \frac{1}{n_{\text{ph}}} \quad \text{[185–187]. Its value in water is } \alpha_0 = 42^\circ, \text{ with } n_{\text{ph}} = 1.33. \text{ Notice here that } n_g \text{ and } n_{\text{ph}} \text{ have similar values but are not equal.}
\]

The distance \( x_1 \) and time \( t_e \) can be calculated as the joint solutions of two separate constraints, as illustrated in Fig. 4.3. The spatial constraint is

\[
x_2^2 = r^2 + x_1^2 - 2x_1 r \cos \theta, \quad (4.2)
\]

which is satisfied by all points along the solid blue line of the muon track. The time constraint is

\[
x_1 + n_g x_2 = c(t - t_0), \quad (4.3)
\]

which is satisfied by all points along the green curve for which the total time — accumulated as a muon for a distance \( x_1 \) and as a photon for a distance \( x_2 \) — is \( t - t_0 \). If \( n_g = 1 \), this curve would be an ellipse with foci at the points associated with \( t_0 \) and \( t \); instead, it is a fourth-order polynomial, and we show a relevant section.

The joint solutions are defined by a quadratic equation in \( x_1 \), obtained by combining the constraints:

\[
\left[ \frac{1}{n_g^2} - 1 \right] x_1^2 + 2 \left[ \vec{r} \cdot \hat{\mu} - \frac{c(t - t_0)}{n_g^2} \right] x_1 + \left[ \frac{c^2(t - t_0)^2}{n_g^2} - r^2 \right] = 0. \quad (4.4)
\]

This is the same as Eq. (4.3) in Ref. [151]; we provide more details on the origin and solutions of this equation. In principle, there could be zero, one, or two solutions. Because every observed photon is emitted at some point on or close to the muon track, there should always be at least one real solution. In Sec. 4.3.2, we show that numerical issues can make it appear that there are none. The Super-K procedure is to measure the coefficients in this equation and solve for \( x_1 \), keeping all solutions that are real and fall into a reasonable range.

The Super-K reconstruction method is compatible with the properties of showers, because it is approximately true that all the light is emitted from a point moving along a straight line. The longitudinal spread of particles at one instant of a shower is \( \sim 0.1 \text{ m} \). For an electromagnetic shower, the transverse extent is also \( \sim 0.1 \text{ m} \); for a hadronic shower, it can be \( \sim 1 \text{ m} \). Finally, typical muon track deflections are small, coincidentally \( \sim 0.1 \text{ m} \) over the height of the ID. As we discuss below, the typical resolution for shower reconstruction is of order a few meters, so these effects are negligible.

This method is powerful because it accounts for all of the observed Cherenkov light. For relativistic muons, a photon is emitted at a fixed angle \( \alpha = \alpha_0 \) relative to the muon track; in this case, the emission point of the photon could also be obtained from a simpler linear equation, e.g., Eq. (4.5). (An earlier Super-K paper [188], on atmospheric neutrinos, reconstructed the muon light profile assuming that all emission was at the Cherenkov angle relative to the muon.) However, for electrons, which can be significantly deflected, the angle \( \alpha \) varies, and the full quadratic equation is needed. The major shortcoming of this method,
in either the quadratic or linear case, is that it neglects correlations between PMT hits, as discussed in detail in Sec. 4.3.5.

As we have shown, the Super-K reconstructed light profiles are inconsistent with what we expect from a shower (or any known process). Yet, at first glance, the Super-K reconstruction method looks correct. To understand the differences between the real and reconstructed light profiles, we take a closer look at the nature of solutions of Eq. (4.4).

4.3.2 Understanding the Reconstruction Solutions

To demonstrate how reconstruction works, we first simulate the Cherenkov light pattern that Super-K observes on the ID walls from muons and their secondaries. We define the $z$ axis to point in the direction along the muon track. For every PMT hit on the walls, Super-K can measure its position $z = \vec{r} \cdot \hat{\mu}$ and time $t$. By light pattern, we mean the $(z, t)$ plane filled by all the PMT hits from one muon and its secondaries. The azimuthal angle for each PMT hit defines a plane for Fig. 4.3; when the light pattern is constructed, those azimuthal angles are discarded.

To calculate the light pattern, we make some reasonable simplifications; a full study by Super-K will be needed to fine-tune the details. We use a cylinder with the same radius (16.9 m) as the Super-K ID, but take it to be much taller, so that all light is collected on the side walls, instead of the ceiling or floor. We take the muons to be vertically downgoing at the center of the cylinder, so that there is azimuthal symmetry on average. For more general cases where the muon is tilted or shifted from the center, the appearance of Fig. 4.4 changes and we discuss it separately. We use (m, ns) as the units, suppressing their display below. The muon enters the ID at $(0, 0)$.

We generate and propagate Cherenkov photons geometrically with our own codes, ignoring light absorption and scattering. For each track segment ($\sim 1$ cm) in FLUKA charged particle propagation, we effectively propagate light with intensity equal to its length along its Cherenkov cone from the midpoint of the segment.

The Super-K data are discrete in $z$ (all points on the surface of a PMT are taken to be the center of the PMT) but continuous in $t$ (though there is smearing due to time resolution). For computational reasons, it is simpler for us to take $z$ to be near-continuous (bins of width 0.05 m) and $t$ to be discrete (bins of duration 3 ns). For each $z$ value, we calculate $t$ and round it to the nearest bin. If a segment is tilted away from the vertical, we uniformly distribute its light between the minimum and maximum $z$. The discreteness of 3 ns in $t$, which is comparable to the timing resolution of the Super-K PMTs, is roughly equivalent to 1 m in $z$. We discuss resolution further below.

As a check, we generate the light patterns with the Cherenkov light propagation in FLUKA, including light absorption and scattering, and the results are consistent. Furthermore, when we use the Super-K reconstruction method, we recover light profiles similar to
Figure 4.4: The time and position \((z = \vec{r} \cdot \hat{\mu})\) pattern of Cherenkov light on the ID walls for one example of a muon and its secondaries. We simulate an infinitely tall cylinder, such that all the photons hit the side walls instead of the ceiling or floor. The arrival position range is thus larger than the height of the Super-K ID (36.2 m). The intensity scale is approximate; the light from muons is about 1 on the scale. The real muon light profile for this example is shown in Figs. 4.5 and 4.6.

Figure 4.4 is an example of the light pattern produced by a muon and its secondaries. The diagonal band with the highest intensity is due to the muon and the most forward electrons in one moderate shower, a couple of small showers, and some low-energy delta rays (which have \(\langle \cos \theta_z \rangle \sim 0.85\)). The remainder of the intensity, less than 20%, which arrives at given positions at later times, is due to significantly deflected electrons; that in the bottom left corner of the figure is due to very deflected electrons that produce light near the ceiling of the detector, where the muon cannot.

How much of this Cherenkov intensity (per bin of time and position) can be detected? The first impression shows blocks of size 1 m, though a zoom-in reveals the 0.05-m bins; both have height 3 ns. Because 1 m of a charged particle corresponds to \(\sim 10^3\) PMT hits, Super-K should be able to detect some light from such blocks with intensities \(\gtrsim 10^{-3}\) (or from 0.05-m bins with intensity \(\gtrsim 10^{-2}\)), assuming each is integrated over 3 ns.

The pattern in Fig. 4.4 from a muon (or any track segment along the \(z\) axis) can be understood from simple arguments. The setup is shown in Fig. 4.3, but here we assume a vertical central muon. The photons emitted at a point \(x_1\) have

\[
z = x_1 + 16.9 \cot \alpha_0 = x_1 + 19,
\]  
(4.5)
and
\[ t = \left( x_1 + \frac{16.9 n g}{\sin \alpha_0} \right) / c = \frac{x_1}{c} + 118, \]  
(4.6)

where 16.9 (m) is the Super-K ID radius and \( \alpha_0 \) is the Cherenkov angle. (For noncentral or nonvertical muons, these and the following expressions can be generalized by changing 16.9 to \( r \sin \theta \).) The offsets correspond to the position shift and time delay for light to reach the walls after the muon first enters the ID. These equations combine to give the pattern
\[ z = c t - 16.9 \left( \frac{n g}{\sin \alpha_0} - \cot \alpha_0 \right) \]  
(4.7)
in Fig. 4.4. This line is broadened to the left, into a band, due to finite detector time and position resolution.

The pattern in Fig. 4.4 from deflected electrons also has a characteristic shape. For deflection by an angle \( \theta_z \), the minimum and maximum \( z \) for the propagated photons are \( x_1 + 16.9 \cot(\alpha_0 \pm \theta_z) \). In a shower, there are many electrons in a short distance, some with very large deflections. For light emitted at all angles from a single point \( x_1 \), the complete pattern is a hyperbola,
\[ (z - x_1)^2 - \frac{c^2(t - t_e)^2}{n_g^2} = -16.9^2, \]  
(4.8)
placed to the left of the line defined by the muon. The lowest point of the hyperbola, \( z_{\text{low}} \), comes from light that travels perpendicular to the wall, which reveals the point of emission through \( x_1 = z_{\text{low}} \). The right-hand side of the hyperbola is populated by light from electrons aligned close to the muon track; the left-hand side by light that is moving upward in the detector, due to very deflected electrons. Because shower electrons are forward-peaked (\( \langle \cos \theta_z \rangle \sim 0.8 \)), the intensity on the hyperbola falls as the electron deflection increases. Outside the range of Fig. 4.4, the Cherenkov intensity is nonzero but negligible.

For other muon positions or orientations, the appearance of Fig. 4.4 changes. For a noncentral but vertical muon, the line from the muon light turns into a band. In this case, photons emitted at the same point but at different azimuthal angles travel different distances to the wall. Consequently, for a fixed \( z \) value on the wall, it gets hit by photons emitted at different positions along the muon track, and they take different times to reach \( z \). For nonvertical muons, the width of the band varies because a nonvertical muon can be considered to be many small tracks of noncentral vertical muons. These effects do not change our results because our reconstructions are based on Fig. 4.3 and Eq. (4.4), which are fully general for each PMT hit. We obtain good results for other muon positions and orientations. In effect, for each range of azimuthal angle and height in detector coordinates, the pattern of PMT hits looks like that shown in Fig. 4.4.

The key to understanding Fig. 4.4 — and hence the reconstruction method — is electron
deflections. We quantify these by the discriminant of Eq. (4.4),
\[ \Delta = \frac{4 \times 16.9^2}{\sin^2 \alpha} \left( \cos \alpha - \frac{1}{n_g} \right)^2, \tag{4.9} \]
which determines the nature of the solutions (for central vertical muons). If the phase
and group velocities were identical, \( \Delta \) would be zero for photons emitted by muons. For
these, \( \Delta \simeq 1 \), much smaller than typical values for electrons. To simplify the discussion, we
approximate \( \Delta \simeq 0 \) for muon light.

Most electrons are quite forward (\( \alpha \simeq \alpha_0 \)), so \( \Delta \) is usually small; because measured PMT
hits correspond to physical solutions, \( \Delta \) must be positive. When an electron is aligned with
the muon, \( \Delta = 0 \) and the two solutions merge, corresponding in Fig. 4.3 to the green curve
from Eq. (4.3) being tangential to the blue muon line from Eq. (4.2). When an electron is
deflected, \( \Delta > 0 \) and there are two real solutions, as in the example shown in Fig. 4.3. As
\( \Delta \) increases, the two real solutions split further apart. Although both are physical, one is
correct and one is not, and these cannot be distinguished on an event-by-event basis. The
Super-K reconstruction method keeps both solutions if they are within a reasonable range,
which leads to a problem of overcounting PMT hits (about 35% in the example of Fig. 4.4).

The typically small discriminant amplifies the effects of the detector time and position
resolution. The measured \( \Delta \) can become negative, corresponding to no real solutions, due to
shifts in the measured quantities used in the coefficients of Eq. (4.4). In Fig. 4.3, the green
curve would be slightly displaced from the blue muon line, with no crossings; in Fig. 4.4,
the PMT hits would be slightly to the right of the line defined by the muon. The Super-K
reconstruction method discards such cases, which leads to a problem of undercounting PMT
hits (about 40% in the example of Fig. 4.4).

These numerical problems also mean that true solutions depend sensitively on the mea-
sured values of \((z, t)\). In Fig. 4.3, the near-straightness of the green curve means that slight
movements of it or the blue muon line lead to large changes in the solutions. In Fig. 4.4,
it is difficult to separate hyperbolas with different emission points \( x_1 \) by looking at their
right-hand sides, where the Cherenkov intensity is greatest. More quantitatively,
\[ x_1(z, t) \simeq x_1(z_0, t_0) + \frac{2.6}{\sqrt{\Delta}}(ct - z)(\delta z - c\delta t), \tag{4.10} \]
where \( \delta z \) and \( \delta t \) describe how incorrect the values of \((z, t)\) are. When \( \Delta \) is small, the error
term scales as \( \sim 20/\sqrt{\Delta} \sim 0.5|\cos \alpha - \cos \alpha_0|^{-1} \) m, which can be several meters for typical
shower electrons. This is significantly larger than the PMT position or time resolution
because of the near-cancellation in \( \Delta \). (As we show in Sec. 4.3.3, when \( \Delta \) is near zero, we
can solve a linear equation instead of the quadratic.) Importantly, this tells us that the best
reconstructions come from the worst electrons, i.e., those with the largest deflections and \( \Delta \)
values.
The nature and precision of the solutions can also be affected by the presence of hadronic showers. For these, transverse displacements of some shower particles can be \( \sim 1 \) m from the muon track, especially for large showers. This means that \( \Delta \) values are shifted compared to the case with no deflection. This can be seen from the fact that there are more negative \( \Delta \) values and they can have larger absolute value, compared to photon hits from electromagnetic showers. The effect is small enough that we can ignore it here, but large enough that it could help identify hadronic showers, which are rare but which produce nearly all isotopes.

With a better understanding of the solutions, we now have insights as to why the Super-K reconstructed profile looks very different from real shower profiles. We next consider how to improve their method.

### 4.3.3 Improving the Reconstruction Method

The exploration in Sec. 4.3.2 reveals how the Super-K reconstruction method works, as well as three improvable limitations. First, when \( \Delta \) is large, taking both solutions includes wrong information and overcounts PMT hits. Second, when \( \Delta \) is negative due to detector resolution, taking zero solutions ignores correct information and undercounts PMT hits. Third, when \( \Delta \) is small, the sensitivity of the solutions to detector resolution dilutes better information.

These limitations result in reconstructed muon light profiles with distorted shapes and inaccurate shower energies. When the shower energy is small, the current method might not be able to localize the shower. Multiple showers cannot be resolved either.

Our goal for improving the reconstruction method is to get an accurate muon light profile. This includes locating the correct shower peak position, getting the correct shower shape and shower energy, and resolving multiple showers. We improve the Super-K method by addressing its three limitations. First, when \( \Delta \) is large, we show how to select the better solution (Improvement 1). Second, when \( \Delta \) is negative, we show how to repair it and recover a solution (Improvement 2). Third, when \( \Delta \) is small, we show that, though these solutions help reconstruct the complete light profile, it is best to set them aside when defining the showers (Improvement 3).

Figure 4.5 shows (in gray shade) the Cherenkov light profile from a simulated muon and its secondaries. Using this specific example, we calculated the \((z, t)\) data shown in Fig. 4.4; here we use that data as if they were observed, attempting to reconstruct an accurate light profile from it.

In this example, the total muon energy loss is 11 GeV. There is a medium-sized shower (about 4 GeV, as can be seen from its area) located near 10 m, a smaller shower near 5 m, and possibly some smaller ones further along the muon track. These are all quite typical in appearance, with the smaller showers being harder to recognize. These particular showers
Figure 4.5: Shower reconstruction with refinement of real solutions. The gray shaded shape is the real (simulated) light profile used to produce the example light pattern in Fig. 4.4. The black line is the result of the reconstruction using the Super-K method. For the red line, we keep only the better one of the two solutions.

are electromagnetic; there are harmless isotopes produced by gamma rays at around 5 m and 30 m. As explained before, the light outside the shower regions is from the muon and low-energy delta rays. It may look like there are larger fluctuations in the muon and delta-ray light than in Fig. 4.1, but this is only because the overall $y$ scale is smaller due to this shower being smaller.

We choose this example because the biggest shower has only moderate energy and because there are two showers close to each other. It is a good test of how well the reconstruction works, both in terms of getting the correct shape of the largest shower and of resolving the small showers.

Figure 4.5 also shows (black line) the result obtained when we use the Super-K reconstruction method. The largest shower is found at the right position, which is why the new Super-K spallation cut works, as shown in Fig. 12 in Ref. [3]. However, the shape of this shower is badly smeared. The area under the black line is comparable to that in the gray shade, but this is an accident, because the Super-K method overcounts and undercounts by roughly equal amounts, as noted. The small showers are not resolved.

Figure 4.5 also shows (red line) the result if we improve the Super-K method by keeping only one solution when there are two (Improvement 1). We first run the Super-K reconstruction method, and record the peak position from the reconstruction. We then run the reconstruction a second time, keeping only the solutions closer to the peak. The red line agrees with the black line near the peak, as expected, but is lower elsewhere because it
is not including wrong solutions and overcounting. Though it defines the showers better, it is still significantly broader than it should be. We note that when the Super-K reconstruction method produces a wrong peak, due to multiple showers or for small showers, Improvement 1 can reinforce it, but does not cause the problem. Improvement 3 can fix the problem because “fake” showers would not have many deflected electrons, as shown in the Appendix.

Next we consider the data for which $\Delta$ is slightly negative due to detector resolution (Improvement 2). Typical values are at worst $-30 \text{ m}^2$ (nominal resolution $\simeq 3 \text{ m}$ [Eq. (4.10)]), corresponding to the level expected from detector resolution. We reconstruct these cases by setting $\Delta = 0$, as would be appropriate for light from the muon or very forward electrons. Because the angle of the particle is known, the quadratic equation reduces to a linear equation, e.g., Eq. (4.5). We use the linear equation only when $\Delta = 0$ (or is reset to be), as the quadratic equation is less sensitive to numerical problems from detector resolution except for the smallest positive values of $\Delta$.

Figure 4.6 shows (green line) the result when we also recover these formerly discarded solutions (all of our improvements of the reconstructed muon profile are cumulative.) This profile is a better match in the peak and especially the baseline to the input in the gray shade than even the red line in Fig. 4.5. There is no longer undercounting of light from undeflected particles, such as the muon itself. Importantly, the area under the green line now matches that in the gray shade. However, the shower peak is still too wide, and no secondary showers are identifiable. Because the green line traces the nonshowering part of the light profile well, it can be used to estimate the energy of the largest shower from its area above the baseline; at this stage of refinement, imperfect precision increases the width of the shower and decreases its height, but conserves its area.

Finally, we focus on the photons that provide the most precise information on the positions of showers (Improvement 3). From Eq. (4.10), these are the ones with large $\Delta$. We choose $\Delta > 100 \text{ m}^2$, corresponding to a nominal resolution of 2 m [Eq. (4.10)]. This comes at a price of keeping only $\sim 10\%$ of the PMT hits, corresponding to $\sim 1 \text{ GeV}$. We solve the quadratic equation, keeping only the solution closest to the shower peak as determined with the Super-K method. We correct the normalization of the blue line by adding a constant baseline of 1 for a muon and by setting the shower energy above the baseline to match that of the green line.

Figure 4.6 also shows (blue line) the result obtained using only the most deflected electrons. The agreement with the input shown in the gray shade is excellent. Compared to previous results, it is much narrower, localizing showers better. Only this method clearly defines multiple showers. We added in the muon baseline to facilitate comparison, but the underlying method ignores the light from the muon and most of its low-energy delta rays. That is, it focuses on the light in showers, where nearly all the isotopes are made.
Figure 4.6: Shower reconstruction with two more improvements. The gray shaded shape is the real (simulated) light profile. For the green line, we repair unphysical data to recover muonlike solutions that were previously discarded. For the blue line, we select only the light from electrons with large deflections to focus on reconstructing only the showers; we add 1 to account for the muon light.

We show all three improvements in this order to best explain the physics. In practice, the first step is Improvement 3, which is to pick out the most deflected electrons. Next is Improvement 1, which is to select only one solution for each PMT hit (for the most deflected electrons). Lastly, one can follow Improvement 2 to get the correct total energy, then scale the profile from Improvement 3+1 to the correct energy. However, one can also skip Improvement 2, and get the total energy simply by counting the total number of PMT hits, then scaling the profile to the correct energy.

We have demonstrated that the Super-K reconstruction technique can be significantly improved, leading to an accurate muon light profile, even when there are multiple showers. However, there are some complications regarding practical implementation, which we discuss next.

4.3.4 Towards Practical Implementation

So far we have assumed that Super-K can measure the position and time of each detected photon within the precision noted in Sec. 4.3.2. However, this is not always possible with the present electronics. Here we discuss the implications and how to achieve the aim of shower reconstruction anyway.

A PMT hit is the basic observable and must be defined carefully. In Super-K, it is defined by the total number of detected photons within a time window and the time of
just the first photon. The number of detected photons is determined by the accumulated charge of the photoelectrons produced. In Super-K, the time window is $\sim 400$ ns (Michael Wilking, private communication; Michael Smy, private communication). As assumed above, the position and number of detected photons are well defined, but the individual times are not, which reduces the available information.

This effect is important for reconstructing muon-induced showers in Super-K. The light yield of a vertical throughgoing muon is high, corresponding to several detected photons per PMT, and more if there are large showers. As shown in Fig. 4.4, the light from the muon always arrives at a given PMT before that from a shower. Because of this, most PMTs lose the timing information on the light from showers. Despite this, Super-K found reasonable reconstructions in Ref. [26], where they weighted the solutions corresponding to each PMT by the total number of detected photons.

Much of the data needed for reconstruction are not affected by this limitation. The key is to identify cases where light from the muon does not reach the PMTs. The most significant reason is due to geometry. For vertically downgoing muons, the most common case, their Cherenkov light cannot reach the PMTs in roughly the top half of the detector. This can be seen in Fig. 4.4; the height of the ID is 36.2 m, and the muon light begins only at a depth of 19 m. We emphasize that the PMTs in the top half of Super-K can detect photons from showers anywhere in the detector. Indeed, the further the direction of the shower light is away from that of the muon light, the better. Another reason is due to fluctuations. Some PMTs that could have been reached by the muon Cherenkov light will not be triggered, and these will properly register late-arriving light.

To check the effects of the timing limitations, we constructed a second simulation, which is a more faithful representation of Super-K. (We do not use this simulation for our main results because it complicates the discussion of the underlying physics.) The simulated region follows the true Super-K ID geometry with the ceiling and the floor. Individual PMTs are mounted on the ID walls with realistic sizes and spacing. We record each photon hit with its total charge and first-hit time, as opposed to treating photoelectrons individually. For the reconstruction, we repeat the Super-K method and our improvements. For Improvement 3, not only do we select the photons with large deflection, but also hits on the ceiling and in the top half of the detector, where no muon light is expected. Our reconstructed profiles reasonably trace the true profiles and can pick out showers occurring even near the bottom of the detector. Thus we are confident that the properties of the PMT electronics will not significantly affect our results.

Longer term, the ability to reconstruct showers could be improved by installing new electronics that allow for pulse-shape discrimination, or at least enough information to separate detected photons that arrive a few tens of ns apart. New technologies for Cherenkov light detection with excellent position and time resolution are extremely promising for
improving shower reconstruction [189–191].

In the near term, the most promising possibility is to go beyond the framework of the Super-K reconstruction method and our improvements, and take advantage of the ideas proposed in the following subsection.

4.3.5 Towards Better Reconstruction Methods

The Super-K reconstruction method, including our improvements, works reasonably well. However, it has fundamental shortcomings. It neglects the correlations between different photons from the same charged particle, i.e., the Cherenkov ring pattern. It neglects the correlations between different electrons emitted from the same position, i.e., the shower angular distribution. And it neglects the correlations between electrons emitted from different positions, i.e., the shower longitudinal profile.

Better methods should be possible. Here we sketch three promising ideas, each for a different energy range; it may be possible to combine them. A good reconstruction needs only to provide the number of relativistic charged particles accompanying the muon, and some information about their angular distribution, each in bins of size $\sim 0.5$ m along the muon track. The muon and the shower each produce a lot of light, $\sim 7000$ PMT hits per GeV, which provides a lot of information for such modest goals. We have had encouraging conversations with Super-K collaborators about specific codes that could be adapted to this purpose, such as fiTQun [192, 193] (private communication, Michael Wilking) and MS-fit [194] (private communication, Michael Smy), if a pure enough sample of hits can be obtained.

To exploit the correlations between photons in the same Cherenkov ring, one must connect the solutions from separate PMTs. Consider a vertically downgoing muon passing through the center of the detector (the considerations generalize). The Cherenkov ring from the muon is a circle of uniform intensity moving down the detector walls. Charged particles in a shower are arrayed in a small, thin, concave bunch centered on the muon. The light from forward electrons adds to that from the muon, but the light from each deflected electron makes a tilted ellipse that intersects the circle from the muon at only two points. When we fit only one PMT hit at a time, it is as if we are azimuthally averaging, turning these ellipses into broad circular bands that blend with the light from each other and that from the forward particles.

For showers of small energy, which are the most important in terms of the frequency of isotope production, it should be possible to simultaneously fit the Cherenkov rings of all charged particles, or at least the most deflected ones. This method may also work for low-energy delta rays.

To exploit the correlations between electrons at the same position, one must take into account the angular distribution of shower particles. Their light follows hyperbolas described
by Eq. (4.8) and clearly visible in Fig. 4.4. We emphasize that the Super-K reconstruction method, even with our improvements, does not exploit these hyperbolic patterns, which is clearly a missed opportunity.

For showers of intermediate energy, it should be possible to fit the portions of the hyperbolas in Fig. 4.4 that can be separated from the light from the muon track. The angular distribution of electrons at a given point along the muon track determines how the intensity varies along the hyperbola. It is probably adequate to focus on the integral of this intensity, which reveals the number of sufficiently deflected electrons at each position.

To exploit the correlations between electrons at different positions, one must take into account the longitudinal shower profile. At present, the values of the reconstructed light from each distance bin along the muon track are independent. This allows fluctuations between different bins that are larger than the intrinsic ones, which likely increases the apparent width of showers. There should be a way to enforce consistency between the values reconstructed for nearby bins.

For showers of large energy, it should be possible to do forward fitting with a template for a shower of unknown energy and position along the muon track, assuming something about the average angular distribution of shower particles. As shown in Fig. 6 in Ref. [3], the intrinsic shower fluctuations at 100 GeV are minimal and those at 10 GeV are moderate; this method may work to even lower energies.

With these or other new methods based on the physics of showers, we are confident that the quality of the reconstructed light profiles can be significantly improved, resolving much smaller showers and multiple showers per muon. This will allow much sharper cuts on spallation isotopes.

4.4 Muon Profile Likelihood

Our goal is to improve spallation background rejection in Super-K, i.e., the separation of spallation decays from neutrino signal events. Currently, Super-K uses spallation likelihood functions that take variables describing a candidate signal event and return a probability that it is a spallation decay.

So far our discussions have been within the framework of the Super-K likelihood function for their DSNB analysis [26], which is based on finding the peak position of a muon light profile. Our work in previous sections shows how to measure this peak better.

In this section, we propose a new framework. We build a spallation likelihood function based on our faithfully reconstructed shower profiles. We quantify its improvement to Super-K spallation cuts.

There is an important distinction between constructing a likelihood function and applying it. When constructing a likelihood, one always knows which primary muon made a
particular spallation isotope, whereas when applying a likelihood, one does not know which
muon to associate a particular event with. We explain the first part in Sec. 4.4.1 and the
second in Sec. 4.4.2.

4.4.1 Spallation Likelihood Functions

In Super-K, solar neutrinos have a low event rate. Intrinsic radioactivity backgrounds
dominate at low energy (< 6 MeV); spallation backgrounds dominate at high energy (6–
18 MeV). Both neutrino events and radioactive backgrounds are uncorrelated with cosmic-
ray muons, and we refer to them as random events.

A Super-K spallation likelihood \( L(C, M) \) evaluates how likely it is that a candidate event
\((C)\) is correlated with a muon \((M)\). The larger \( L \), the more likely that this \( C \) is made by
this \( M \), i.e., is a spallation decay. Otherwise, it is likely an uncorrelated random event.
(Below, we directly define likelihood functions; Super-K analyses use the logarithm of the
likelihood, which is equivalent.)

A good likelihood function reflects the physics of how muons make spallation isotopes.
(Though well motivated on general grounds, the Super-K likelihood functions are empiri-
cal.) There are several steps to build this function. First, one picks variables describing
a candidate event that are statistically different for spallation decays and random events.
Some obvious choices are the differences in time and transverse position between a can-
didate event and its parent muon as well as the muon energy loss. A basic assumption
that Super-K adopts, which we keep, is that these variables are independent, i.e., that the
likelihood function can be factorized.

Second, one selects a spallation decay sample along with their parent muons. In simu-
lation, this is easy. In practice, Super-K selects candidate events that are close to muons
in time and space, and that have high energy (to avoid radioactive backgrounds). This is
sufficient to select an almost pure spallation sample, due to their high rate.

Third, one selects a random sample with uncorrelated muons. In simulation, we simply
produce candidate events that are uniform in time and space, and randomly pair them
with muons. In practice, Super-K pairs candidate events with muons that follow, instead
of precede, candidate events in time.

Finally, one builds every component in a likelihood function. For each variable, one
measures the distributions of this variable for the spallation event sample and the random
event sample. Then, each likelihood component is the ratio of the distributions of the
spallation sample relative to the random sample.

The first likelihood function that Super-K developed, which is still used for solar neutrino
analyses [14], is

\[
L_{\text{flat}} = F_t(t) \cdot F_{L_{\text{trans}}}(L_{\text{trans}}) \cdot F_q(Q_{\text{res}}).
\]  (4.11)
Here $t$ and $L_{\text{trans}}$ are the time difference and the transverse distance between a spallation decay and a muon track, and $Q_{\text{res}}$ is the radiative energy loss of the muon (measured by subtracting the light of a minimum-ionization muon from the total). We can understand the behaviors of these components based on shower physics. $F_t$ decreases due to the exponential decays of spallation isotopes. $F_l$ decreases due to the exponential decrease in secondary particle, and thus spallation isotope, density away from the muon track. $F_q$ increases due to excess energy loss producing more secondary particles and spallation isotopes. Their functional forms are given in Refs. [14, 180].

The likelihood function in Eq. (4.11) does not directly reflect shower physics. The $Q_{\text{res}}$ variable includes energy loss from all showers and low-energy delta rays along a muon track. It can be close to the energy of the largest shower if that shower is very energetic, but most commonly it sums over comparable small showers and low-energy delta rays. In addition, this likelihood does not include shower position information.

A new likelihood function Super-K recently developed, which is applied to the DSNB analysis [26], is

$$L_{\text{peak}} = F_t(t) \cdot F_l(L_{\text{trans}}) \cdot F_q'(Q_{\text{peak}}) \cdot F_l'(L_{\text{long}}).$$

(4.12)

Here $Q_{\text{peak}}$ is the total light in the central 4.5 m of the reconstructed peak and $L_{\text{long}}$ is the longitudinal distance (along the muon track) between the peak and the candidate event. $F_l'$ decreases with respect to the absolute value of $L_{\text{long}}$ because spallation isotopes are most frequently produced in the biggest showers. $F_q'$ increases because secondary particle path lengths, and hence spallation production, are proportional to shower energy. Their functional forms are given in Ref. [151].

The likelihood function in Eq. (4.12) improved upon that in Eq. (4.11) and reflects some shower physics, though this was not recognized as the reason. The variable $Q_{\text{peak}}$ would be a good measure of the shower energy if the reconstruction were perfect, but it is not accurate, as we explained earlier. This likelihood keeps the peak position of the biggest shower from reconstruction but discards the shape of the shower and smaller showers.

It is easy to see how our work on improving muon light profile reconstruction improves the efficiency of this likelihood. First, we can measure the true shower energy without overcounting or undercounting problems (see Sec. 4.3.3). Second, the functional form of $F_l'$ gets sharper (see Fig. 12 of Ref. [3]), which more clearly separates spallation decays from random events.

To fully utilize the information about showers in the reconstructed muon light profiles, we propose a new likelihood,

$$L_{\text{shower}} = F_t(t) \cdot F_l(L_{\text{trans}}) \cdot F_z(z).$$

(4.13)

Here $z$ is the position along the muon track from where it enters the ID. For a muon with
Figure 4.7: Comparison of the $L_{\text{long}}$ or $z$ component of the three different likelihood functions, normalized to equal area. The $y$ axis unit is the Cherenkov light intensity, but we also use it for likelihoods because they have arbitrary normalization. The gray shaded region is the real muon light profile, with muon light subtracted. (We cut off the $y$ axis at 5, but the light intensity at 23 m goes to 8.) The red star at 8 m indicates the position of a spallation event.

The likelihood function in Eq. (4.13) fully incorporates information about showers. Spallation production at each position is roughly proportional to the local secondary particle path length, which is roughly proportional to the local light intensity. Random events have a flat position distribution along the muon track. $F_z$ directly reflects how the probability of spallation production varies along a particular muon track.

Figure 4.7 illustrates the term containing $L_{\text{long}}$ or $z$ in these likelihood functions for an example muon. The real muon light profile is shown in gray. There are two showers. Most frequently, the isotope would be associated with the larger one. However, in this case, the isotope is produced in the smaller shower.

To emphasize the shape differences of these three likelihood functions, we normalize them to the same area. $L_{\text{flat}}$ cuts background equally everywhere along the muon track. It cuts events in shower regions too weakly and nonshower regions too strongly. $L_{\text{peak}}$ correctly picks out the biggest shower along the muon track and cuts events in that region with more weight, although its shape does not trace this shower perfectly because the likelihood is from

\[ L_{\text{peak}} \]
an average shower profile. Further, when there are multiple showers, $L_{\text{peak}}$ cuts events in the small-shower regions too weakly. For $L_{\text{shower}}$, the likelihood function is the reconstructed shower profile itself. As shown in this example, it not only traces the large shower well, but it also picks out the small shower. It cuts spallation isotopes with weight proportional to the local shower intensity, which is close to optimal.

### 4.4.2 Efficiency Improvements

We now quantify the improvement of our shower likelihood function over the Super-K likelihood functions. To do so, we need to explain how to apply a cut, i.e., decide whether to discard a candidate event as a spallation decay on the basis of a likelihood test.

When applying a cut to a candidate event, one does not know which muon, if any, is correlated with it. This is different from building a likelihood, where every spallation decay is paired with its parent muon and every random event is paired with an uncorrelated muon.

The first step of applying a cut is thus to build an event likelihood $L_C(C)$ that returns the likelihood of an event being a spallation decay (from any muon). This is done by taking a likelihood function $L(C, M)$ and marginalizing over all muons $\{M_i\}$ that are possibly correlated with this candidate, which in practice are muons in the previous 100 s ($\sim 200$ muons). One calculates $L_i = L(C, M_i)$ for each muon. The maximum value of $L_i$ is then assigned to this candidate event as its event likelihood:

$$L_C(C) = \max_i L(C, M_i). \quad (4.14)$$

Second, one obtains a spallation decay event sample and a random event sample, and finds the distributions of $L_C$ for both samples. The methods to get event samples are as described in Sec. 4.4.1, except that one discards the information about the candidate-muon correlations. Then, one calculates the distributions of the event likelihoods $L_C$.

For a specific likelihood function, the distributions of $L_C$ for the spallation and random samples both have a bump, and drop off at small and large values. By design, the average $L_C$ value for the spallation sample is larger than that for the random sample. However, the two distributions have significant overlap, which is why it is difficult to categorize a candidate as a spallation decay or a random event. Because of the arbitrary normalization of $L(C, M)$, one should not compare $L_C$ distributions for different likelihood functions.

Third, one chooses a value, $L_{\text{cut}}$, that best separates the $L_C$ distributions from the two samples. The choice of $L_{\text{cut}}$ determines its effects on the signal and backgrounds, characterized by deadtime and cut efficiency. Deadtime is the fraction of random events with $L_C > L_{\text{cut}}$, which defines the signal loss. Cut efficiency is the fraction of spallation decays with $L_C > L_{\text{cut}}$, which describes the background rejection. Hence, we want to minimize deadtime while we maximize cut efficiency. For too small a value of $L_{\text{cut}}$, the
deadtime would be unacceptably high. For too large a value of $L_{\text{cut}}$, the cut efficiency would be unacceptably low. An optimal value $L_{\text{cut}}$ must be chosen to maximize the signal detection significance. For Super-K flat likelihood function, the cut efficiency and deadtime for the optimal $L_{\text{cut}}$ are about 90% (10% background remaining) and 20% for their solar neutrino analyses [14, 180].

Finally, one applies the cut to the real data sample, rejecting events with $L_{\text{C}} > L_{\text{cut}}$.

Now we can compare the efficiencies of different likelihood functions. We vary the $L_{\text{cut}}$ value for each likelihood, obtaining pairs of deadtime and cut efficiency values. The optimal $L_{\text{cut}}$ value would correspond to specific values.

To better separate the factors that contribute to the differences between likelihood functions, we make some simplifications. First, to show the maximum improvement possible due to better reconstruction methods, we take the real (simulated) muon light profiles instead of the reconstructed ones. Second, to fairly compare the difference between the peak and shower likelihood functions, we add an improved peak likelihood that we explain below. Third, we include only single throughgoing muons. Lastly, our spallation samples have only spallation decays, whereas in Super-K analyses there are some random events. Despite these simplifications, our results for the flat likelihood are consistent with the Super-K measurements and the differences among different likelihoods should be reasonably accurate.

Figure 4.8 shows the deadtime and cut efficiency for the three likelihood functions. To emphasize the improvement, we show background remaining, which is $(1 - \text{cut efficiency})$, on the $x$ axis. The flat [Eq. (4.11)], peak [Eq. (4.12)], and shower [Eq. (4.13)] likelihoods
take the functional forms we defined, with components taken from Super-K measurements or our definitions. To take into account the fact that we use real muon light profiles, we show the peak improved likelihood, which is based on the Super-K peak likelihood formula, but we adjust $F'_l(L_{\text{long}})$ (both shown in Fig. 12 in Ref. [3]), assuming that the peak position can be measured perfectly.

To make the comparisons specific, we compare likelihoods at fixed deadtime ($\approx 20\%$), which focuses on background reduction. (One could also compare at fixed cut efficiency, which focuses on signal gain.)

Going from the flat likelihood to the Super-K peak likelihood, the background remaining decreases from 0.12 to 0.09. This shows how the method of Ref. [26] used for the DSNB analysis could benefit Super-K solar studies by focusing cuts on regions where the muon light profile peaks. With a better peak localization, as our techniques could provide, the improvement would be to 0.07. Finally, with our new shower likelihood, the complete improvement would be from 0.12 to 0.05. Thus, it should be possible to reduce backgrounds by more than a factor of 2 with the results we present in this paper. This can be combined with other cuts we have suggested or will present in forthcoming papers.

Our proposed new shower likelihood function, based on better reconstructed muon light profiles, could substantially reduce backgrounds. It takes variables directly from each muon light profile, so it should be easy to implement.

In addition to the single throughgoing muons we consider, there are three other classes of muons identified by Super-K that are subdominant but relevant [26]. Stopping muons only make isotopes when $\mu^-$ undergo nuclear capture [3, 95], and we discuss cuts in Ref. [3]. Corner-clipping muons are just a category of throughgoing muons where reconstruction is more difficult. Isotopes will be produced in the FV only when there is a shower that enters the ID (excess light in the outer detector may help identify large showers), because the lateral extent of a shower ($\lesssim 1$ m) and thus of isotope production is less than the thickness of the ID-FV shielding (2 m) [2, 3]. For multiple muons, also known as muon bundles, pairs of muons produced in the same atmospheric shower are the most common case [195–197]. Higher-multiplicity events can be cut aggressively without appreciable deadtime. Our reconstruction method could be adapted to deal with pairs, treating them together when the separation is $\lesssim 1$ m and singly when it is larger, along with straightforward adjustments for the amount of light and number of showers expected. In summary, we see no barriers to adapting our methods to implement a complete background-rejection program in Super-K.

4.5 Conclusions

Muon-induced spallation backgrounds are a major source of background for low-energy neutrino detection. Nevertheless, a complete picture of how these spallation isotopes are
produced and a strong enough background rejection method have been lacking. We are conducting a series of studies intended to provide a comprehensive theoretical understanding of how muons make spallation isotopes and to propose better ways to reject them.

In our previous papers [2, 3], we found that almost all spallation isotopes are produced by secondary particles, and that almost all secondary particles are made in muon-induced showers. Our calculations agree with Super-K measurements on the total spallation yield and other data. We also explained an empirical cut that Super-K developed for their DSNB analysis [26]. However, one discrepancy remained: The Super-K reconstructed muon light profiles show prominent bump features, which are grossly inconsistent with shower physics.

In this paper, we show that the observed bump features are indeed caused by muon-induced showers. The reason that they look too wide and short compared to showers can be traced back to the Super-K muon light profile reconstruction method.

We suggest ways to improve the Super-K reconstruction method. By measuring the position and time for every PMT hit, Super-K solves a quadratic equation for the emission position of the photon along a muon track. However, due to the electron deflection in showers and detector resolution, the quadratic equation could have zero, one, or two solutions for one PMT hit, and the solutions could be shifted from their true values. We propose ways to improve this by picking out one solution when there are two, recovering one solution when there seem to be zero, and focusing on the PMT hits that give solutions closest to the true values. We show that our improvements could lead to almost perfectly reconstructed muon light profiles.

We then propose a new spallation likelihood function, based on better reconstructed methods, that fully exploits the information contained in muon light profiles. We demonstrated that it, combined with a better reconstruction method, can reduce the remaining background by a factor of 2 compared to the Super-K DSNB analysis cut, and even more compared to their solar analysis cut.

Our results could be easily adopted by Super-K for their solar neutrino and DSNB analyses. The background rejection improvement could be especially dramatic for solar neutrinos, where the current cut does not even take advantage of the muon light profile peaks, much less the full understanding of shower physics.

The techniques we developed will benefit other neutrino experiments. Our results have immediate applications for other water Cherenkov detectors, e.g., Hyper-Kamiokande [142], which will be shallower than Super-K. And, because our reconstruction method does not depend on the geometry of the PMTs, it could be applied to muon reconstruction in high-energy neutrino telescopes like IceCube [198], where fluctuations in shower energy along muon tracks are used to estimate muon energy. Finally, our reconstruction technique does not depend on the direction of the light, so our results could be adapted for scintillator detectors [see Eq. (4.8) for isotropic light emission], especially in large-scale next-generation
detectors such as JUNO [199].

4.6 Supplemental Material

4.6.1 Additional reconstruction examples

Here we show examples of muon light profile reconstruction for a variety of other cases.

Figure 4.9 shows a muon event with only small showers. There are two showers, at \( \sim 2 \) and 16 m. The Super-K profile using the Super-K method does not reveal either shower, and is mostly noise. Our reconstructed profile, however, successfully picks out both showers.

Figure 4.10 shows a muon event with moderate but comparable showers, at \( \sim 12 \) and 23 m (and smaller ones at \( \sim 2 \) m and 30 m). The Super-K reconstructed profile is reasonable for one shower, poor for the others, and has a false shower in the middle. Our reconstructed profile reconstructs all four showers clearly.

Figure 4.11 shows a muon event with a hadronic shower. This is a relatively clean event. Both profiles have the correct peak position, and trace the shower shape. The Super-K profile is more smeared out. Our reconstructed shower is not as sharp as large in other examples due to the larger lateral displacement of charged particles in hadronic showers.

In summary, these examples demonstrate the better performance of our reconstruction for small, multiple and hadronic showers.

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Figure 4.9: Shower reconstruction example—only small showers. **Left panel:** The gray shaded shape is the real (simulated) light profile. The black line is the result of the reconstruction using the Super-K method. The blue line is the result of our improvements. **Right panel:** The time and position pattern of Cherenkov light on the ID walls for this muon event.

Figure 4.10: Shower reconstruction example—two comparable showers. Descriptions as in Fig. 4.9. The only difference is that we use a bin size of 1 m in the left panel to reduce fluctuations.
Figure 4.11: Shower reconstruction example—hadronic showers. Descriptions as in Fig. 4.9
Chapter 5

Echo Technique to Distinguish Flavors of Astrophysical Neutrinos

The flavor composition of high-energy astrophysical neutrinos is a rich observable. However, present analyses cannot effectively distinguish particle showers induced by $\nu_e$ versus $\nu_\tau$. We show that this can be accomplished by measuring the intensities of the delayed, collective light emission from muon decays and neutron captures, which are, on average, greater for $\nu_\tau$ than for $\nu_e$. This new technique would significantly improve tests of the nature of astrophysical sources and of neutrino properties. We discuss the promising prospects for implementing it in IceCube and other detectors.

The contents of this chapter were published in Ref. [200].

5.1 Introduction

High-energy astrophysical neutrinos, long sought, were recently discovered by the IceCube Collaboration [17, 18, 20, 53, 59, 60]. Their energy spectrum provides important clues about extreme astrophysical sources as well as neutrino properties at unexplored energies. However, pressing mysteries remain.

Exploiting the flavor composition — the ratios of the fluxes of $\nu_e + \bar{\nu}_e$, $\nu_\mu + \bar{\nu}_\mu$, and $\nu_\tau + \bar{\nu}_\tau$ to the total flux — offers crucial additional clues. In the nominal scenario, a composition of $(\frac{1}{3} : \frac{2}{3} : 0)_S$ at the source is transformed by neutrino vacuum mixing to $(\frac{1}{3} : \frac{1}{3} : \frac{1}{3})_\oplus$ at Earth [27, 28]. Even for arbitrary flavor composition at the source, the maximal range of flavor composition at Earth with only standard mixing is surprisingly narrow [29], making deviations sensitive indicators of new physics [201–227].

So far, IceCube measurements of the flavor composition mostly separate muon tracks — made primarily by charged-current (CC) $\nu_\mu + \bar{\nu}_\mu$ interactions — from particle showers — made by all other interactions. A significant limitation is their poor ability to distinguish
between CC interactions of $\nu_e$ and $\nu_\tau$ (unless noted, $\nu_l$ refers to $\nu_l + \bar{\nu}_l$).

### 5.2 Synopsis of the paper

We propose a new technique to break this $\nu_e$-$\nu_\tau$ degeneracy, one that could work for a wider range of energies than existing ideas (Glashow resonance [228–230], double pulses [56], double bangs [27], and lollipops [55]).

We introduce two new shower observables. In showers, low-energy muons and neutrons are produced; after delays, the muons decay and the neutrons capture. We call the collective Cherenkov emission from the many independent decays and captures the **muon echo** and the **neutron echo**. We show that the echoes are brighter for $\nu_\tau$-initiated than for $\nu_e$-initiated showers, which could allow them to be distinguished on a statistical basis.

Our focus is pointing out new observables to help solve the important problem of flavor identification. The technical aspects of implementation require experimental expertise. Nevertheless, in a preliminary evaluation, grounded in the measured properties of IceCube, we find the detection prospects promising.

Figure 5.1 shows that the present $\nu_e$-$\nu_\tau$ degeneracy in IceCube elongates the contours of the measured flavor composition [18]. It also shows how detecting echoes could refine these measurements, probing the flavor composition better than the maximal range with standard mixing [29], which would lead to powerful conclusions.
5.3 High-energy neutrino signatures

At present, IceCube identifies neutrino-initiated events only as tracks and showers, for which the Cherenkov light appears to emanate from approximate lines and spheres. Tracks are caused by muons, which travel up to $\sim 10$ km in ice [17], due to their low interaction and decay rates. Showers are caused by all other neutrino-induced particles and extend only $\sim 10$ m in ice [17], due to the high interaction and decay rates of their constituent particles.

Neutrinos produce secondaries through deep-inelastic scattering [16, 64, 231]. A neutrino interacts with a nucleon $N$ via the CC channel $\nu_l + N \rightarrow l + X$ or the neutral-current (NC) channel $\nu_l + N \rightarrow \nu_l + X$, where $l = e, \mu, \tau$, and $X$ represents hadrons. A fraction $(1 - y)$ of the neutrino energy goes to the final-state lepton; the remaining fraction $y$ goes to the final-state hadrons. The inelasticity distribution peaks at $y = 0$ and has an average $\langle y \rangle \approx 0.3$ at 100 TeV, for both $\nu$ and $\bar{\nu}$, CC and NC.

Tracks are produced by $\nu_\mu$ CC interactions plus 17% of $\nu_\tau$ CC interactions where the tau decays to a muon [232].

Showers are produced by all other neutrino interactions. For $\nu_e$ CC interactions, the electron- and hadron-initiated showers combine, and their sum energy equals the neutrino energy. For $\nu_\tau$ CC interactions, the tau decays promptly, so again the showers combine (when the tau does not decay to a muon); the neutrino energy estimate is slightly biased because $\sim 25\%$ of its energy is lost to outgoing neutrinos from tau decay. For NC interactions of all flavors, the hadron-initiated shower carries a fraction $y$ of the neutrino energy; because of the steeply falling neutrino spectrum, NC interactions are subdominant in the total shower spectrum [63]. (This is also true for mis-identified $\nu_\mu$ CC interactions that appear to be a shower event because the track is missed [222].)

These points explain the basic features of the IceCube results in Fig. 5.1. Because there are track events, the $\nu_\mu$ component of the flux must be nonzero; because there are shower events, the sum of the $\nu_e$ and $\nu_\tau$ components must be nonzero. The similarity of $\nu_e$- and $\nu_\tau$-initiated events makes the contours nearly horizontal; the degeneracy is weakly broken because increasing the $\nu_\tau/\nu_e$ fraction increases the number of tracks and decreases the shower energies. With present methods, improvement requires much larger exposure [29].

5.4 Electromagnetic versus hadronic showers

The key to our new method is understanding the low-energy physics underlying high-energy showers [2–4, 156, 162, 163, 170, 175].

When showers are developing, particles multiply in number while decreasing in energy. An electromagnetic shower starts out with electrons, positrons, and gamma rays and stays composed predominantly of them; there is usually a small fraction of pions and nucleons produced by photonuclear processes. A hadronic shower starts out with pions and nu-
cleons, and then builds up a progressively larger fraction of electromagnetic particles as prompt $\pi^0 \rightarrow \gamma\gamma$ decays deplete $\sim 1/3$ of the remaining hadronic energy with each shower generation.

Shower development ends when the average particle energy is low enough that the particle- and energy-loss rates exceed the particle-production rates. At that point, the most abundant particles in all showers are $\sim 100$-MeV electrons and positrons, which produce most of the prompt Cherenkov light. Pions carry only $\sim 10\%$ of the energy in hadronic showers and $\sim 1\%$ in electromagnetic showers. However, they are the key to separating electromagnetic and hadronic showers.

### 5.5 New shower observables

At the end of shower development, charged pions come to rest by ionization; then $\pi^-$ capture on nuclei and $\pi^+$ decay to $\mu^+$. The $\mu^+$ decay with a lifetime of $2.2\ \mu s$, producing $e^+$ with $\sim 35$ MeV. The collective Cherenkov light from these positrons is our first new observable: the *muon echo*.

Separately, neutrons lose energy by collisions until they reach thermal energy. They eventually capture on hydrogen, with a timescale of $\sim 200\ \mu s$, producing $2.2$ MeV gamma rays. (In seawater, $33\%$ of neutrons capture on Cl; the emitted gamma rays have $8.6$ MeV [233], making the neutron echoes more visible.) The gamma rays Compton-scatter electrons to moderate energies, producing Cherenkov light. This collective emission is our second new observable: the *neutron echo*.

We simulate showers and subsequent echoes using the FLUKA Monte Carlo software (version 2011.2c-4) [84, 85]. We inject high-energy electrons or positrons to simulate electromagnetic showers and charged pions to simulate hadronic showers.

Figure 5.2 shows the averaged time profile of a 100-TeV hadronic shower. Because the features happen on very different timescales, it is appropriate to analyze their light yield $L$ in bins of log time. Accordingly, we plot $dL/d\log t \propto t \ dL/dt$; this makes the height of the curve proportional to its contribution to the integrated light yield. The echo shapes are exponentials with the respective timescales. The echoes are well-separated from the prompt shower and from each other.

Figure 5.2 also shows that the echoes have low intensities: the muon echo has $\sim 3 \times 10^{-3}$ of the prompt shower energy and the neutron echo has $\sim 6 \times 10^{-4}$. The first number results from the facts that $10\%$ of hadronic shower energy goes to pions, $10\%$ of those pions are $\pi^+$ that come to rest and decay, and $30\%$ of the pion decay energy goes to positrons from muon decays. The second number results from the facts that there are about 10 times more neutron captures than muon decays, that the capture energy is about 20 times smaller, and that the Cherenkov efficiency is about 3 times smaller.
Figure 5.2: Time evolution of the light yield of a hadronic shower simulated with FLUKA, following injection of a 100-TeV charged pion. The shaded bands are exponentials with the respective timescales. For an electromagnetic shower of the same prompt energy, the echoes are $\sim 10$ times smaller.

The points above carry over for electromagnetic showers, except for a crucial difference: the pions carry only $\sim 1\%$ of the shower energy as opposed to $\sim 10\%$. Thus the echo intensities are expected to be $\sim 10$ times higher in hadronic showers than in electromagnetic showers.

Figure 5.3 shows that there are indeed about 10 times as many muon decays and neutron captures in hadronic showers. This difference is much larger than the intrinsic fluctuations of these numbers. Because the number of decays and captures, and, therefore, the light coming from them, grows linearly with shower energy, this factor-of-10 difference between electromagnetic and hadronic showers is present at all energies. The yields may have an overall shift of up to a factor of 2 due to hadronic and nuclear uncertainties [2, 82, 83, 86], but this can be calibrated by external measurements [115, 181, 190, 234] or in situ.

5.6 Separating $\nu_e$ and $\nu_\tau$

We now examine how echoes can be used to help identify the flavors of neutrino-induced showers. In realistic neutrino interactions, the differences in the echoes are less stark than above.

Showers initiated by $\nu_e$ are mostly electromagnetic because the outgoing electron typically carries more energy than the final-state hadrons. But showers initiated by $\nu_\tau$ are mostly hadronic because, in addition to the shower from the final-state hadrons, 67\% of tau decays are hadronic. (NC showers are purely hadronic.)
We consider flavor separation at fixed shower energy, as opposed to fixed neutrino energy, to make contact with experiment. We simulate neutrino interactions with appropriate energies to give $E_{\text{sh}} = 100$ TeV, including 10% energy resolution [54]. For NC interactions, we mimic the final-state hadrons by directly injecting charged pions at the shower energy.

Figure 5.4 shows how the numbers of muon decays per shower are distributed for different neutrino interaction channels. As expected, $\nu_e$ CC showers produce fewer muons than $\nu_\tau$ CC showers.

The basics of the distributions in Fig. 5.4 can be understood easily. For pure electromagnetic showers, the peak would be at $\sim 500$ decays; it would be narrow because most pions are produced late in the shower and the fluctuations are mostly Poissonian. For pure hadronic showers, the peak would be at $\sim 8000$ decays; it would be broad because there are large fluctuations in how much energy goes into $\pi^0$ in the first few shower generations. The shapes shown in Fig. 5.4 depend also on the $y$ distributions for neutrino interactions. For $\nu_e$ CC events, the distribution is substantially broadened because the differential cross section $d\sigma/dy$, while peaked at $y = 0$, has a substantial tail. For $\nu_\tau$ CC events, there is a slight shift to the left, due to the 17% of tau decays to muons.

The results in Fig. 5.4 make it possible to distinguish $\nu_e$ and $\nu_\tau$ on a statistical basis.

We next estimate the sensitivity to flavor composition using the echoes from an ensemble of events, assuming perfect detection efficiency.

First, we use the results in Fig. 5.4 to generate the muon decay distributions for each flavor, assuming an equal flux of $\nu_l$ and $\bar{\nu}_l$, and NC to CC event ratios consistent with a power-law spectral index of 2.5 [18]. Next, for an assumed flavor composition, we randomly
sample the number of muon decays for each shower in an ensemble of 100 showers of $E_{\text{sh}} = 100$ TeV. Then, we treat the flavor composition $f_{\nu_e,\oplus}$ and $f_{\nu_\tau,\oplus}$ as free parameters ($f_{\nu_\mu,\oplus} = 1 - f_{\nu_e,\oplus} - f_{\nu_\tau,\oplus}$) and use an unbinned maximum-likelihood procedure to find their best-fit values. We generate $10^3$ different realizations of the shower ensemble, and find the average best-fit values and uncertainties of $f_{\nu_e,\oplus}$ and $f_{\nu_\tau,\oplus}$. Further details are in Appendices 5.9.1 and 5.9.2.

Figure 5.1 shows the predicted sensitivity on $f_{\nu_e,\oplus}$ and $f_{\nu_\tau,\oplus}$, assuming equal $\nu_e$ and $\nu_\tau$ content, i.e., a composition of the form $(x : 1 - 2x : x)_{\oplus}$, where $x$ varies in $[0, 0.5]$. The vertical shape of the band shows that the sensitivity to $f_{\nu_e,\oplus}$ and $f_{\nu_\tau,\oplus}$ does not depend on the $\nu_\mu$ content. (Because our method is only weakly sensitive to $f_{\nu_\mu,\oplus}$, we suppress its uncertainty in the plot.)

Our results are conservative. The sensitivity improves slightly with shower energy; see Appendix 5.9.3. Assuming perfect detection efficiency, the sensitivity is comparable whether we use muon echoes only, neutron echoes only, or both; see Appendix 5.9.4. It is also comparable, or better, for other choices of input parameters; see Appendix 5.9.5.

5.7 Observability of the echoes

Echo detection depends on how the echo light yield compares to that from ambient backgrounds and detector transients. These quantities are detector-dependent, and we use IceCube as a concrete example.

The echoes are faint, but they are well localized, which enhances their visibility. In space, like the parent shower, they are concentrated among only the few photomultiplier
tubes (PMT) on a single string that are closest to the neutrino interaction vertex [58]. In
time, they occur $\sim 2.2 \mu s$ and $\sim 200 \mu s$ after the prompt shower. These timescales require
long-time data collection, made possible by the recent development of the HitSpooling
technique, which can go to hours for infrequent events [235]. In direction, the shower light
is beamed forward but the echo light is isotropic. Light scattering makes the shower more
isotropic and increases its duration [54], which could partially obscure the muon echo.

The total light yield of a shower in IceCube is $\sim 100$ detected photoelectrons (p.e.) per
TeV [17]. For 100 TeV, the muon echo in a hadronic shower is expected to yield $\sim 30$ p.e.
and the neutron echo $\sim 6$ p.e. The low p.e. counts set the energy threshold for our method.

Ambient backgrounds in IceCube do not eclipse the echoes. For an average p.e. noise
rate of $\sim 500$ Hz per PMT [236], the expected backgrounds in 2 $\mu s$ and 200 $\mu s$ are only
$\sim 10^{-3}$ and $\sim 10^{-1}$ p.e. per PMT, respectively. (Even with correlated noise, due to nuclear
decays near the PMT, the backgrounds will be small in all but a few PMTs, and those
will be identifiable [237].) And the cosmic-ray muon rate in IceCube is 3 kHz [17], so the
probability of a muon lighting up several specific PMTs in the short time between shower
and echo is small.

A serious concern is the detector transient called afterpulsing, where a PMT registers
late p.e. with total charge proportional to the initial signal (the shower) and with a time
profile characteristic to the PMT. For the IceCube PMTs, the muon echo will compete with
an afterpulse feature of relative amplitude $\sim 10^{-2}E_{\text{sh}}$ near 2 $\mu s$ [236]; though larger than
the echo, it is not overwhelmingly so. Encouragingly, the neutron echo, though smaller, is
late enough that afterpulsing seems to be negligible.

In summary, the prospects for observing echoes are promising, and they improve with
shower energy. Doing so may require changes in detector design or in PMT technology [238];
these considerations may shape the design of IceCube-Gen2 [239], KM3NeT [240, 241],
and Baikal-GVD [242]. With multiple nearby PMTs [239, 241, 243], it may be possible
to reconstruct individual events, dramatically improving background rejection. The final
word on the observability of the echoes will come from detailed studies by the experimental
collaborations.

5.8 Conclusion

The rich phenomenology contained in the flavor composition of high-energy astrophysical
neutrinos cannot be fully explored due to the difficulty of distinguishing showers initiated
by $\nu_e$ versus $\nu_\tau$ in neutrino telescopes. To break this degeneracy, we have introduced two
new observables of showers: the delayed, collective light, or “echoes,” from muon decays
and neutron captures. This light reflects the size of the hadronic component of a shower,
and it is stronger in $\nu_\tau$-initiated than $\nu_e$-initiated showers.
Figure 5.1 shows the promise of our method for IceCube. With assumptions of 100 showers and perfect detection efficiency, echo measurements would improve the separation of $\nu_e$ and $\nu_\tau$ by a factor of $\sim 9$ over present measurements. That is comparable to the estimated sensitivity attainable with the present technique after more than 50 years of exposure of the next-generation detector IceCube-Gen2, assuming it will have an effective area 6 times larger than IceCube.

The applications of tagging hadronic showers via muon and neutron echoes extend beyond flavor discrimination. The technique could improve shower energy reconstruction, by folding in the probability of a shower being electromagnetic or hadronic. And, at the considered energies, the echoes are shifted forward along the shower direction by $\sim 5$ m from the shower peak. If this shift can be detected, it would improve the poor angular resolution of showers [54].

High-energy neutrino astronomy has just begun. We are still learning the best ways to detect and analyze astrophysical neutrinos. We should pursue all potentially detectable signatures, edging closer to finding the origins and properties of these ghostly messengers.

5.9 Supplemental Material

In the main text, we showed how detecting muon echoes can improve discrimination between $\nu_e$-initiated and $\nu_\tau$-initiated showers. We showed results using 100-TeV showers and a flavor composition of the form $(x : 1 - 2x : x)_{\odot}$. Here we provide more details on the statistical method and show how the results depend on choices of inputs.

In Appendix 5.9.1, we present the underlying formalism for flavor discrimination per shower. In Appendix 5.9.2, we apply it to an ensemble of showers. In Appendix 5.9.3, we discuss flavor discrimination at other shower energies. In Appendix 5.9.4, we discuss neutron echoes. In Appendix 5.9.5, we show sensitivity results for other input choices.

To simplify the notation, we explicitly show the shower energy $E_{sh}$ dependence when defining a quantity, and suppress it otherwise. In the probability definitions, we show $\nu$ CC cases explicitly; NC and $\bar{\nu}$ cases have similar definitions, with CC replaced by NC, and $\nu$ replaced by $\bar{\nu}$.

5.9.1 Flavor discrimination for one shower

We calculate the probability that an observed shower, containing $N_\mu$ muon decays, was initiated by a neutrino $\nu_l$, of definite flavor $l = e, \mu, \tau$.

The main observable of a shower is its energy $E_{sh}$, which is proportional to the total collected light. Because the detector energy resolution is narrow, we simply take it to be flat in the range $[0.9, 1.1] E_{sh}$. 
Using Bayes’ theorem, the probability that a shower with energy $E_{sh}$ and $N_\mu$ muon decays was initiated by a $\nu_l$ is

$$P_{\nu_l|N_\mu}(E_{sh}) = \frac{P_{CC_{\nu_l}} N_{CC_{\nu_l}} + P_{NC_{\nu_l}} N_{NC_{\nu_l}}}{\sum_{\alpha=e,\mu,\tau} N_{CC_{\nu_\alpha}} + N_{NC_{\nu_\alpha}}} \cdot \left[ P_{CC_{\nu_l}} P_{CC_{\nu_\alpha}} + P_{NC_{\nu_l}} P_{NC_{\nu_\alpha}} \right].$$

(5.1)

Here, $P_{\nu_l}(E_{sh})$ is the probability that a shower with energy $E_{sh}$ is produced by the CC interaction of a $\nu_l$, which we detail below, while $P_{CC_{\nu_l}}(E_{sh})$ is the probability that said shower yields $N_\mu$ muon decays, which is calculated via FLUKA simulations and shown in Figs. 5.4 and 5.7 for different shower energies.

The probability $P_{\nu_l}^{CC}$ is defined as

$$P_{\nu_l}^{CC}(E_{sh}) = \frac{N_{CC_{\nu_l}}}{\sum_{\alpha=e,\mu,\tau} N_{CC_{\nu_\alpha}} + N_{NC_{\nu_\alpha}}} \cdot \left[ N_{CC_{\nu_l}} + N_{NC_{\nu_l}} \right],$$

(5.2)

where $N_{CC_{\nu_l}}(E_{sh})$ is the number of $\nu_l$-initiated showers generated by CC interactions. The denominator in Eq. (5.2) is the total number of showers initiated by all flavors of neutrinos and anti-neutrinos.

To calculate the number of showers, we use the “theorist’s approach” [244], assuming perfect detector efficiency at the relevant energies. The final results on flavor discrimination are affected by only the relative, not the absolute, event rates from different flavors. We consider a flux $F_{\nu_l}$ of $\nu_l$ (in units of GeV$^{-1}$ cm$^{-2}$ s$^{-1}$ sr$^{-1}$) arriving at the detector, which contains $N$ target nucleons. The flux already includes any attenuation due to propagation in the Earth. In observation time $\Delta t$ with detection solid angle $\Delta \Omega$, the number of detected $\nu_l$-initiated CC showers is

$$N_{CC_{\nu_l}}(E_{sh}) = N \cdot \Delta t \cdot \Delta \Omega \cdot \int_0^\infty F_{\nu_l}(E_\nu) \cdot \sigma_{\nu_l}^{CC}(E_\nu) \cdot g_{\nu_l}^{CC}(E_\nu, E_{sh}) \, dE_\nu,$$

(5.3)

where $E_\nu$ is the neutrino energy and $\sigma_{\nu_l}^{CC}$ is the neutrino-nucleon CC cross section [16, 64, 231]. The function $g_{\nu_l}^{CC}$ is the probability that a neutrino with energy $E_\nu$ creates a shower with energy $E_{sh}$; it is different for each flavor.

- In $\nu_e$ CC interactions, all of the neutrino energy is deposited in the electromagnetic and hadronic showers. Accordingly, we define

$$g_{\nu_e}^{CC} = \begin{cases} 1, & \text{if } E_\nu \in [0.9, 1.1] E_{sh} \\ 0, & \text{otherwise} \end{cases}.$$  

(5.4)

- In $\nu_\tau$ CC interactions, the outgoing tau has numerous decay modes. All of them have outgoing neutrinos, which carry away energy and do not appear in the shower, so that $E_{sh} \lesssim E_\nu$. On average, the outgoing neutrinos carry away 40% of the tau energy, or
25% of the primary neutrino energy. For simplicity, we make $g_{\nu_{\tau}}^{CC}$ nonzero only in the energy range $E_\nu \in [0.9, 1.1]E_{sh}/0.75$. Since 17% of tau decays are into muons and neutrinos, without a shower, we estimate

$$g_{\nu_{\tau}}^{CC} = \begin{cases} 0.83, & \text{if } E_\nu \in [0.9, 1.1]E_{sh}/0.75 \\ 0, & \text{otherwise} \end{cases}. \quad (5.5)$$

- In NC interactions, the energy deposited in the shower is the energy of the final-state hadrons, i.e., $E_{sh} = yE_\nu$. For the shower energy to lie within 10% of $E_{sh}$, the value of $y$ must lie in the range $[y_{\text{min}}, y_{\text{max}}] \equiv [0.9, 1.1]E_{sh}/E_\nu$. Hence, we define

$$g_{\nu_{l}}^{NC}(E_\nu) = \frac{\int_{y_{\text{min}}}^{y_{\text{max}}} d\sigma_{\nu_{l}}^{NC}(E_\nu, y) dy}{\int_{0}^{1} d\sigma_{\nu_{l}}^{NC}(E_\nu, y) dy}, \quad (5.6)$$

where $d\sigma_{\nu_{l}}^{NC}/dy$ is the $y$ probability distribution for NC interactions [231]. However, because hadron-initiated showers carry a small fraction $y$ of the neutrino energy, and because the neutrino flux is steeply falling, NC showers are subdominant to CC showers [63].

- In $\nu_{\mu}$ CC interactions, the outgoing muon leaves an identifiable track. We exclude these events by setting

$$g_{\nu_{\mu}}^{CC} = 0 \quad (5.7)$$

We have assumed that no track is mis-identified as a shower; otherwise, the value of $g_{\nu_{\mu}}^{CC}$ would be set to the probability of mis-identification. As with NC events, these would be subdominant in the shower spectrum.

We write Eqs. (5.1)–(5.3) in a more useful way. Consider an all-flavor astrophysical neutrino flux $\propto E_\nu^{-\gamma}$ and flavor ratios at Earth ($f_{e,\oplus} : f_{\mu,\oplus} : f_{\tau,\oplus}$), such that the flux of $\nu_l$ is $F_{\nu_l} = f_{l,\oplus}F_0E_\nu^{-\gamma}$, with $F_0$ the normalization of the flux. With this, Eq. (5.3) becomes

$$N_{\nu_{l}}^{CC}(E_{sh}) = \mathcal{N} \cdot \Delta t \cdot \Delta \Omega \cdot F_0 \cdot f_{l,\oplus} \cdot I_{\nu_{l}}^{CC}(E_{sh}), \quad (5.8)$$

with the shorthand

$$I_{\nu_{l}}^{CC}(E_{sh}) \equiv \int_{0}^{\infty} E_\nu^{-\gamma} \cdot \sigma_{\nu_{l}}^{CC}(E_\nu) \cdot g_{\nu_{l}}^{CC}(E_\nu, E_{sh}) dE_\nu. \quad (5.9)$$

Finally, using Eqs. (5.8) and (5.9), and assuming equal flavor ratios for neutrinos and anti-
neutrinos, Eq. (5.1) becomes

\[ P_{\nu|N_{\mu}}(E_{sh}) = \frac{f_{e,\oplus} \left[ P_{CC}^{\nu_{\mu}|\nu_{\ell}} I_{\nu_{\ell}}^{CC} + P_{NC}^{\nu_{\mu}|\nu_{\ell}} I_{\nu_{\ell}}^{NC} \right]}{\sum_{\alpha=e,\mu,\tau} f_{\alpha,\oplus} \left( P_{CC}^{\nu_{\mu}|\nu_{\alpha}} I_{\nu_{\alpha}}^{CC} + P_{NC}^{\nu_{\mu}|\nu_{\alpha}} I_{\nu_{\alpha}}^{NC} \right)} \]  

(5.10)

The probability that the shower with \( N_{\mu} \) muon decays was created by a \( \nu_{\ell} \) or a \( \bar{\nu}_{\ell} \) is simply \( P_{\nu|N_{\mu}} + P_{\bar{\nu}|N_{\mu}} \).

Figure 5.5 shows this probability computed at \( E_{sh} = 100 \) TeV, assuming a diffuse astrophysical neutrino flux with spectral index \( \gamma = 2.5 \) and a flavor composition of \( \left( \frac{1}{3} : \frac{1}{3} : \frac{1}{3} \right)_{\oplus} \), compatible with IceCube results [18]. The neutrino is more likely to be a \( \nu_{e} \) if there are fewer muon decays and a \( \nu_{\tau} \) if there are more decays. The probability that the shower is from a \( \nu_{\mu} \) NC interaction (not shown) reaches at most 10\%, at large values of \( N_{\mu} \).

5.9.2 Flavor discrimination for an ensemble of showers

We use the results from Appendix 5.9.1 to infer the \( f_{e,\oplus} \) and \( f_{\tau,\oplus} \) flavor ratios of an ensemble of showers. We first explain how we generate the artificial shower ensemble; then we show how to infer their flavor ratios.

To generate an ensemble of showers with energy \( E_{sh} \), we first assume a neutrino flux with spectral index \( \gamma = 2.5 \) and “real” values for the flavor ratios \( \left( f_{e,\oplus}^{\nu_{\ell}} : f_{\mu,\oplus}^{\nu_{\ell}} : f_{\tau,\oplus}^{\nu_{\ell}} \right) \). We then use the probability distribution functions of the number of muon decays for each channel, \( P_{\nu_{\mu}|\nu_{\ell}}^{CC} \) and \( P_{\nu_{\mu}|\nu_{\ell}}^{NC} \) (shown in Figs. 5.4 and 5.7), to construct the total probability distribution of

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Figure 5.5: Probability that one neutrino-induced shower was generated by a \( \nu_{e} \) (via either CC or NC) or \( \nu_{\tau} \), as a function of number of muon decays. The curve for \( \nu_{\mu} \) is calculated but not shown.
Figure 5.6: Distributions of muon decays for an ensemble of 100 showers of 100 TeV, for different choices of flavor composition \((f_{e,\oplus} : f_{\mu,\oplus} : f_{\tau,\oplus})\), reflecting the central value and width of the band in Fig. 5.1.

muon decays associated to that flux, by summing over all flavors and interaction channels:

\[
P_{\mu,\text{tot}} (N_{\mu}; E_{\text{sh}}, \{f_{\alpha,\oplus}\}) = \sum_{\alpha=e,\mu,\tau} [P_{N_{\mu} | \nu_{\alpha}} \cdot P_{\nu_{\alpha}} (f_{\alpha,\oplus}) + P_{N_{\mu} | \bar{\nu}_{\alpha}} \cdot P_{\bar{\nu}_{\alpha}} (f_{\alpha,\oplus})] + [\nu_{\alpha} \rightarrow \bar{\nu}_{\alpha}].
\]

Figure 5.6 shows the total muon decay distribution for \(E_{\text{sh}} = 100\) TeV, for three choices of flavor composition. The distribution for our nominal case \((\frac{1}{3} : \frac{1}{3} : \frac{1}{3})\) \(\oplus\) has a saddle shape, peaked at low number of decays due to the sharp distribution of the \(\nu_{e}\) CC channel. The height of this peak increases with \(f_{e,\oplus}\).

We use the above distribution to randomly sample the number of muon decays for each shower, that is, we obtain \(N_{\mu,i}\) for \(i = 1, \ldots, N_{\text{sh}}\). These are our “real” data. We choose \(N_{\text{sh}} = 100\), consistent with near-future expectations for IceCube.

Merely to illustrate the flavor separation power given this sample size, we include binned data for this choice in Fig. 5.6. The points and error bars show the expected number of showers per bin and its 1\(\sigma\) Poissonian fluctuation. The power of flavor discrimination using muon echoes hinges on the ratio of the number of showers with few muon decays — e.g., \(N_{\mu} < 3000\) — to the number of showers with many muon decays — e.g., \(N_{\mu} > 6000\). A higher ratio drives \(f_{e,\oplus}\) up and \(f_{\tau,\oplus}\) down, and vice versa.

For our actual analysis, we recover the flavor ratios \(f_{\alpha,\oplus}\) of the ensemble via an unbinned maximum likelihood approach. The likelihood function for a test flavor composition
Figure 5.7: Normalized distributions of the numbers of muon decays per shower of energy 10 TeV and 1 PeV for different neutrino interaction channels. Note the changes in x-axis scale compared to Fig. 5.4.

\begin{equation}
(f_{\nu,e}, f_{\mu,\oplus}, f_{\tau,\oplus}), \text{ with } f_{\mu,\oplus} \equiv 1 - f_{\nu,e} - f_{\tau,\oplus}, \text{ is }
\end{equation}

\[ L(f_{\nu,e}, f_{\tau,\oplus}) = G(f_{\mu,\oplus}) \prod_{i=1}^{N_{sh}} P_{\mu,tot}(N_{\mu,i}; f_{\nu,e}, f_{\tau,\oplus}). \] (5.11)

The Gaussian term, $G(f_{\mu,\oplus})$, constrains the muon component from deviating too much from its true value, assuming it can be measured from a separate track analysis. We choose the $1\sigma$ width of the Gaussian to be 0.12, consistent with the present IceCube measurement [18]. The maximum value of the likelihood determines the best-fit values of $f_{\nu,e}$, $f_{\tau,\oplus}$, and $f_{\mu,\oplus} = 1 - f_{\nu,e} - f_{\tau,\oplus}$. To estimate the uncertainty on this value, we repeat the maximum likelihood procedure using 1000 random realizations of the real data. Figure 5.1 shows the best-fit values and uncertainties on $f_{\nu,e}$ and $f_{\tau,\oplus}$ that result from this procedure, assuming ensembles of $N_{sh} = 100$ showers each and real flavor ratios $f_{\nu,e}^{r} = f_{\tau,\oplus}^{r} = (1 - f_{\mu,\oplus}^{r})/2$, with $f_{\mu,\oplus}^{r}$ varying in the range $[0, 1]$.

5.9.3 Results for different energies

In the main text, we consider showers of 100 TeV; the normalized distribution of number of muon decays for this shower energy is shown in Fig. 5.4.

Figure 5.7 shows the distributions at 10 TeV and 1 PeV. The same general shapes and behavior of the curves is seen at all energies: $\nu_e$-initiated CC showers have appreciably fewer muon decays than $\nu_\tau$-initiated CC showers and NC showers. The main change is in
the intensity of the muon echo, which scales roughly linearly with shower energy.

As the shower energy changes, there are moderate changes in the results. The value of $\langle y \rangle$ decreases with increasing energy, which means that $\nu_e$-initiated CC showers become more leptonic. And the $y$ distributions for $\nu$ and $\bar{\nu}$ become more similar at higher energies, and, therefore, so do their muon decay distributions. Therefore, the separation between $\nu_e$ and $\nu_\tau$ becomes cleaner at higher energies. This is evidenced by contrasting the panels in Fig. 5.7.

5.9.4 Results for neutron echoes

Like the muon echo, the neutron echo is a product of the hadronic component of a shower.

Figure 5.8 shows that the number of muon decays and the number of neutron captures is tightly correlated on an event-by-event basis. Because of this, the probability distributions of the numbers of neutron captures behave similarly to those of muon decays (Figs. 5.4 and 5.7), except for a scaling of the x-axis by a factor of about 10.

If we were to incorporate neutron echoes in our sensitivity estimate, Eq. (5.11) would have an extra term $\prod_{i=1}^{N_{sh}} P_{n,\text{tot}} (N_{n,i}; f_{e,\oplus}, f_{\tau,\oplus})$ on the right-hand side, with $N_{n,i}$ the number of neutron captures in each shower of the ensemble. However, the distribution of number of neutron captures, $P_{n,\text{tot}}$, is essentially just $P_{\mu,\text{tot}}$ scaled up by a factor of 10. Therefore, adding it to the likelihood would not alter the best-fit values of $f_{e,\oplus}$ and $f_{\tau,\oplus}$ or their uncertainties.

This is true from a theoretical perspective. However, from an experimental perspective, neutron echoes are attractive because there seems to be less PMT afterpulsing at late times.
Finally, there is a third possible post-shower signal — the spallation echo — coming from the collective Cherenkov light from beta decays of long-lived ($\sim 0.1–10$ s) unstable nuclei. These isotopes, which are a background in low-energy neutrino detectors, are produced more efficiently in hadronic than electromagnetic showers, by a factor $\sim 10$ [2–4]. While the spallation echo is not observable in IceCube or similar detectors due to ambient backgrounds, it might have an application in another context.

5.9.5 Results for other input choices

Figure 5.9 shows the flavor sensitivity, using muon echoes, for three different assumptions of the flavor composition at Earth, including the one shown in Fig. 5.1.

For the choice of flavor composition in Fig. 5.1, the average 1σ uncertainty was 0.07. For $(0 : 2x : 1−2x)\oplus$, with $x \in [0, 0.5]$, the best-fit values lie on the left axis of the plot; only the one-sided 1σ range, of size 0.01, is visible. For $(1−2x : 2x : 0)\oplus$, the best-fit values lie on the right axis of the plot; the one-sided 1σ range, of size 0.04, is visible. These are two extreme choices. Their smaller uncertainties are due to the fact that the total distribution of muon decays of the shower ensemble is dominated by the distribution from either $\nu_e$-initiated or $\nu_\tau$-initiated CC showers. Hence, our nominal choice of flavor composition, in Fig. 5.1, was conservative, as it has the largest uncertainty.

At fixed shower energy, the uncertainty on the $\nu_e$ fraction scales as $\sqrt{N_{\text{sh}}}$, subject to some caveats. When $N_{\text{sh}}$ is small ($\lesssim 20$), the likelihood is basically flat, and one typically cannot break the $\nu_e$-$\nu_\tau$ degeneracy with good precision. When $N_{\text{sh}}$ is large ($\gtrsim 1000$), one should take a narrower prior on the $\nu_\mu$ fraction to reflect its measurement being correspondingly better.

The flavor sensitivity is robust against other input choices. For example, the average 1σ uncertainty is virtually unaffected for a harder neutrino flux of $\gamma = 2$, compared to $\gamma = 2.5$.

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Figure 5.9: Expected precision of our proposed technique for 100 detected showers at 100 TeV, for different assumptions of the flavor composition $f_l$ ($l = e, \mu, \tau$) of astrophysical neutrinos at Earth: (0 : 2$x$ : 1 − 2$x$)$_\oplus$ (left band), (x : 1 − 2$x$ : $x$)$_\oplus$ (central band, same as in Fig. 5.1), and (1 − 2$x$ : 2$x$ : 0)$_\oplus$ (right band), with $x \in [0, 0.5]$. 


[121] A. Empl, R. Jasim, E. Hungerford, and P. Mosteiro. Study of Cosmogenic Neutron Backgrounds at LNGS.


