Reconstruction and Calibration of SNO+ Water

Jie Hu

A Dissertation

Presented to the Faculty

of University of Alberta

in Candidacy for the Degree

of Doctor of Philosophy

Recommended for Acceptance

by the Department of

Department of Physics

January, 2019

Abstract

0.1 Abstract

A neutrino is one of the elementary particles we currently know and is included in the Standard Model (SM). However, some properties of neutrinos can not be described by the SM, which shows clues of the new physics beyond the Standard Model.

SNO+ experiment is planned to explore one of the unknown properties of neutrinos: whether the neutrinos are Majorana particles or Dirac particles.

Acknowledgements

Contents

Abstract **iii**

0.1 Abstract iii

Acknowledgements **iv**

Contents **v**

List of Figures **vii**

List of Tables **viii**

1 Introduction **1**

1.1 Neutrino Oscillation 1

1.2 Majorana Neutrino 1

1.3 Double Beta Decay 2

1.3.1 Status of Double Beta Decay Experiments 3

2 The SNO+ Experiment **5**

2.1 A Description of SNO+ Detector 5

2.1.1 Overview 5

2.1.2 SNO+ Physics Phases 6

2.1.3 Electronics 7

2.1.4 Optics 7

2.1.5 Liquid scintillator 8
2.1.6 Calibration 8

3 Event Reconstruction **10**
3.1 Reconstruction of the SNO+ 10
3.2 Reconstruction Algorithms for Position, Time and Energy of Events in SNO+ 10
3.3 An Alternative Vertex Reconstruction Algorithm for SNO+ 10
3.4 Likelihood Calculation 16
3.5 ^{16}N test 17
3.6 Vertex Reconstruction for the SNO+ Partial-phase 17

4 Partial-filled Scintillator Phase **20**
4.1 Reconstruction of the SNO+ 20
4.2 Reconstruction Algorithms for Position, Time and Energy of Events in SNO+ 20
4.3 An Alternative Vertex Reconstruction Algorithm for SNO+ 20
4.4 Likelihood Calculation 26
4.5 ^{16}N test 27
4.6 Vertex Reconstruction for the SNO+ Partial-phase 27

A Appendix Name **30**

References **31**

List of Figures

3.1 PMT response time as the timing pdf. 12

3.2 PMT angular distribution as the angular response pdf. 12

4.1 PMT response time as the timing pdf. 22

4.2 PMT angular distribution as the angular response pdf. 22

List of Tables

3.1 scintillator α/β timing parameters**??**. 18

4.1 scintillator α/β timing parameters**??**. 28

Chapter 1

Introduction

Neutrinos are one of the elementary particles we currently know and are included in the Standard Model (SM). However, some properties of neutrinos can not be described by the SM, which shows clues of the new physics beyond the Standard Model.

SNO+ experiment is planned to explore one of the unknown properties of neutrinos: whether the neutrinos are Majorana particles or Dirac particles.

Massive neutrinos are discussed ...

1.1 Neutrino Oscillation

Neutrino oscillation was first discovered in 1998. It is the first direct evidence showing that the Standard Model is incomplete.

solar neutrino oscillations

matter effect

1.2 Majorana Neutrino

Dirac equation $(i\gamma^{\mu}\partial_{\mu} - m)\psi = 0$, get coupled equations

The interpretation of the $0\nu\beta\beta$ process is considered as exchanging light Majorana neutrinos. In this case the effective Majorana mass $< m_{ee} >= \sum_{i=1}^{3} |U_{ei}|^2 m_i$ $(i = 1, 2, 3)$,

U_{ei} are the elements of the neutrino mixing matrix for the flavor state ν_e, and m_i are the mass eigenvalues of the mass eigenstates (from (**??**)). The observable quantity is the half-life:

$$(T_{1/2}^{0\nu\beta\beta})^{-1} = G_{PS}(Q,Z)|M_{Nuclear}|^2 < m_{ee} >^2,$$

Majorana found a representation of the γ-matrices as follow:

$$\gamma_M^0 = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \gamma_M^1 = \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}, \gamma_M^2 = \begin{pmatrix} -\sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix}, \gamma_M^3 = -i \begin{pmatrix} \sigma^1 & 0 \\ 0 & \sigma^1 \end{pmatrix}$$

These matrices themselves are pure imaginary.

1.3 Double Beta Decay

For heavy radioactive isotopes with nuclei of even neutron number (N) and even proton number (Z) (called even-even nucleus), beta decay will lead to an odd-odd nucleus which is less stable. For some such isotopes the beta decay is energetically forbidden. In 1935, Maria Goeppert-Mayer pointed out that they can still decay through a double beta decay process: $(Z,A) \to (Z+2,A) + 2e^- + 2\bar{\nu}_e + Q_{\beta\beta}$, where the $Q_{\beta\beta}$ is the released energy. This is called ordinary double beta decay or $2\nu\beta\beta$, which is allowed by the Standard Model and with a typical half-life $T_{1/2} > 10^{19}$ years[**?**].

In 1937, Ettore Majorana proposed that neutral spin-1/2 particles (fermions) can be their own antiparticles[**?**]. If neutrinos have this behaviour, the process called neutrinoless double beta decay ($0\nu\beta\beta$) will also be expected. The Feynman diagrams of $2\nu\beta\beta$ and $0\nu\beta\beta$ are illustrated in Figure **??**.

The interpretation of the $0\nu\beta\beta$ process is considered as exchanging light Majorana neutrinos. In this case the effective Majorana mass $< m_{ee} >= \sum_{i=1}^{3} |U_{ei}|^2 m_i$ $(i = 1,2,3)$, U_{ei} are the elements of the neutrino mixing matrix for the flavor state ν_e, and m_i are the mass eigenvalues of the mass eigenstates (from (**??**)). The observable quantity is the half-life:

$$(T_{1/2}^{0\nu\beta\beta})^{-1} = G_{PS}(Q,Z)|M_{Nuclear}|^2 < m_{ee} >^2,$$

where G_{PS} is the phase space factor and $|M_{Nuclear}|$ is the nuclear matrix element for the physics process describing the $0\nu\beta\beta$ decay process[**?**].

Similar to beta decay, the $2\nu\beta\beta$ process will cause a continuous spectrum in the detector while the $0\nu\beta\beta$ process only has two electrons in the final state, which sum up to give a distinct energy peak. By measuring this exact energy, a detector with high energy resolution is able to search for the $0\nu\beta\beta$ signal from the $0\nu\beta\beta$ decay radioactive isotopes. Diverse technologies have been developed during the past decades. The following section lists some of the mainstream experiments.

1.3.1 Status of Double Beta Decay Experiments

At the time of writing,

$0\nu\beta\beta$ in the range of $10^{25} - 10^{26}$ year,

The GERmanium Detector Array (GERDA) experiment searches for $0\nu\beta\beta$ of ^{76}Ge. The experiment uses bare germanium crystals with an enrichment of up to ~87% ^{76}Ge operated in a radiopure cryogenic liquid argon (LAr). GERDA Phase I had an exposure of 21.6 kg·yr and Phase-II started with 35.6kg from enriched material in December 2015. With combined data of Phase I and Phase II,

a total exposure of 82.4 kg·yr

GERDA reported in 2019 a lower limit half-life of $T^{0\nu}_{1/2}(^{76}\mathrm{Ge}) > 0.9 \times 10^{26}$ years at 90% C.L.[**?**, **?**].

The Enriched Xenon Observatory (EXO) experiment uses 200-kg liquid Xenon (LXe) time projection chamber (TPC) to search for $0\nu\beta\beta$ in ^{136}Xe. In 2011 they observed the half life of double beta decay of ^{136}Xe to be 2.11×10^{21} years and in 2014 they set a limit on $T^{0\nu}_{1/2}(^{136}\mathrm{Xe}) > 1.1 \times 10^{25}$ yr[**?**]. EXO is now upgrading to the next 5-tonne experiment (nEXO) and is expected to reach an exclusion sensitivity of $T^{0\nu}_{1/2}(^{136}\mathrm{Xe})$ to about 10^{28} years at 90% C.L.[**?**].

Also looking into ^{136}Xe, the KamLAND-Zen (ZEroNeutrino) experiment exploits the existing facilities of KamLAND by setting a 3.08-m-diameter spherical inner balloon filled with 13 tons of Xe-loaded liquid scintillator at the center of the KamLAND detector.

liquid scintillator cocktail of 82% decane and 18% pseudocumene by volume, 2.7 g/L PPO.

photocathode coverage of 34%.

Their 2016 results from a 504 kg·yr exposure obtained a lower limit for the $0\nu\beta\beta$ decay half-life of $T^{0\nu}_{1/2}(^{136}\mathrm{Xe}) > 1.07 \times 10^{26}$ yr at 90% C.L. and the corresponding upper limits on the effective Majorana neutrino mass are in the range 61-165 meV[**?**].

The Particle and Astrophysical Xenon Experiment III (PandaX-III) high pressure gas-phase time projection chamber (TPC)

The Cryogenic Underground Observatory for Rare Events (CUORE) experiment searches for $0\nu\beta\beta$ in ^{130}Te. CUORE is a ton-scale cryogenic bolometer array that arranges 988 tellurium dioxide (TeO_2) crystals. CUORE reported first results in 2017 after a total TeO_2 exposure of 86.3 kg·yr. Combined with their early data, they placed a lower limit of $T^{0\nu}_{1/2}(^{130}\mathrm{Te}) > 1.5 \times 10^{25}$ yr at 90% C.L. and $m_{\beta\beta} < (140 - 400)$ meV[**?**].

Chapter 2

The SNO+ Experiment

2.1 A Description of SNO+ Detector

2.1.1 Overview

The SNO+ experiment is located at SNOLAB in Vale's Creighton mine in Sudbury, Ontario, Canada. The deep underground facility of the SNOLAB provides a 2092 ± 6 m flat overburden of rock, which is 5890 ± 94 water equivalent meter (w.e.m). This rock overburden ensures an extremely low rate of cosmic muons passing through the detector. The rate is 0.27 $\mu/m^2/day$, compared to an average flux of about 1.44×10^6 $\mu/m^2/day$ at sea level[1].

The detector has been running since December 2016[**?**],

The SNO+ detector is the successor of the SNO experiment, which makes use of the SNO detector structure.

detector consists of an acrylic vessel (AV) sphere of 12 m in diameter and

5.5 cm in thickness. The AV sphere is concentric within a stainless steel photomultiplier(PMT) support structure (PSUP), with an average radius of 8.4 m. The Hamamatsu 8-inch R1408 PMTs are mounted on the PSUP. 9394 PMTs are looking inward to the AV, giving a 50% effective coverage, while 90 PMTs are looking outward, serving as muon vetos. These two structures are housed in a rock cavity filled with 7000 tonnes of ultrapure water

(UPW) to provide both buoyancy for the vessel and radiation shielding.

main upgrades from SNO to SNO+

2.1.2 SNO+ Physics Phases

The SNO+ detector is designed for multi-purpose measurements of neutrino physics. The experiment will go through three phases[**?**]:

1. Water phase

The AV was filled with about 905 tonnes of ultra pure water (UPW). The detector has been collecting physics data since May 2017.

The main physics goal in this phase is to search for the invisible nucleon decay, which violates baryon number and is a prediction of Grand Unified Theory (GUT). In this decay mode, ^{16}O decays into ^{15}O* or ^{15}O*, which de-excites and produces a γ ray of about 6 MeV.

During the water phase, different types of calibration runs have been taken. The detector responses, systematics and backgrounds are studied. Multiple physics analyses of solar neutrinos, reactor antineutrinos and nucleon decay are going on. The external backgrounds are also measured, which will be the same as the following two phases.

2. Scintillator phase

The AV will be filled with 780 tonnes of liquid scintillator, which is a mixture of linear alkylbenzene (LAB) as a solvent and 2 g/L of 2,5-diphenyloxazole (PPO) as a fluor.

In this phase, the main physics goal is to measure low energy solar neutrinos: the CNO, pep and low energy ^{8}B neutrinos. The pep neutrinos are mono-energetic, with E_{ν}=1.442 MeV and their flux is well predicted by the Standard Solar Model. A measurement of the pep neutrinos will give more information of the matter effects in neutrino oscillations[**?**].

The solar metallicity is the abundance of elements heavier than ^{4}He (called "metal" elements in the context of astronomy). It is poorly constrained and the predictions from different solar models disagree with each other. A measurement of the CNO neutrinos can give the abundance of ^{12}C, ^{13}N and ^{15}O and can thus resolve the metallicity problem[**?**].

Geoneutrino, reactor antineutrino and supernova neutrino detections are additional goals.

A six-month period of scintillator filling and six to twelve months of data-taking are expected for this phase. During the filling, it is planned to operate the partially filled detector at a water level about 4.4 m for about two weeks. This partial filled transition phase is mainly aimed to understand the in-situ backgrounds of scintillator.

3. Tellurium loading phase

In this final phase, 0.5% natural Tellurium by mass will be loaded into the scintillator. Higher loading concentrations would be possible for a further loading plan[4]. The ^{130}Te is a double beta decay isotope. The main purpose in this phase is searching for $0\nu\beta\beta$ in ^{130}Te.

2.1.3 Electronics

PMTs are Hamamatsu model R1408.

a single RG59/U type 75 Ω coaxial cable

19 crates$\times$16 cards$\times$32 channels = 9728 electronics channels.

Each crate processes 16$\times$32 = 512 PMTs. 9605 channels are actually used and among them, 32 channels are reserved for calibration devices and labelled as FEC Diagnose (FECD) channels

During the experiment running, the maintenance of the electronics is always ongoing.

crate controller card (XL3)

analog master trigger system (MTC/A+) ("+" means an upgrade to SNO MTC/A)

digital master trigger system (MTC/D)

the analog waveforms are summed on the MTC/A+ card, then they are digitized

CAEN v1720 digitizer

TUBii trigger utility board pulsers and delays

DAQ

nearline provides a real-time analysis of the data quality,

trigger system PMT Interface Card (PMTIC) Front End Card (FEC)

NHit20 (N20), NHit100 (N100) trigger pulses.

MTC/A has 3 discriminators: LOW, MED and HI.

Global Trigger (GT) the timing and charge from the fired PMT is digitized and stored.

2.1.4 Optics

Optical parameters

timing

attenuation

scattering

laser pulse diffuser, it can run with different wavelengths: 337, 365, 385, 420, 450 and 500 nm. The laserball

2.1.5 Liquid scintillator

Linear Alkyl Benzene (LAB)

The advantages of LAB are:

- It has very low levels of natural radioactive contaminants such as U, Th and K.

  since ionic

- It has a high light yield

- It has fast timing response

  different timing spectrum for α and β events, which enables an $\alpha - \beta$ discrimination.

- It is chemically compatible with AV.

- It is cheap, for

telluric acid (TeA), 1,2-butanediol (BD) N,N-dimethyldodecylamine (DDA) as a stabilisation agent. Te-loaded liquid scintillator (TeLS)

water-based wavelength shifter

2.1.6 Calibration

Calibration source

The ^{16}N source ^{3}H$(p, \gamma)^{4}$He reaction.

the SNO+ Source Manipulator System (SMS) is inherited from the SNO.

A Umbilical Retrieval Mechanism (URM) is used to send the source down to the inner vessel.

The sources are connected to the umbilical.

An umbilical encloses electrical cables, optical fibres and gas lines connected to the source.

A Universal Interface (UI) connecting the URM and the detector, Therefore, sealed environment, which ensures radon gas not leaking into the detector when deploying the source.

-

Chapter 3

Event Reconstruction

.q

3.1 Reconstruction of the SNO+

3.2 Reconstruction Algorithms for Position, Time and Energy of Events in SNO+

3.3 An Alternative Vertex Reconstruction Algorithm for SNO+

A Multi-path Fitter (MPF) framework was developed by the University of Alberta group as an alternative reconstruction algorithm to the SNO+ official fitter. In this framework, fitters for SNO+ water phase (MP Water Fitter), wavelength shifter (MP WLS Fitter), partial-fill phase (MP Partial Fitter) and scintillator phase (MP Scint Fitter) were developed. In SNO+ water phase, the cavity and the AV are both filled with pure water. This is a relatively simple geometry. Therefore, we start with the MP Water Fitter to explain the reconstruction concepts.

First, the fitter throws a random vertex (uniformly distributing) inside the PSUP as a trial vertex. The Class Library for High Energy Physics (CLHEP) is used for creating pseudo-random numbers.

$rand0 = Uniform(0, 1), rand1 = Uniform(-1, 1)$

double ran0 = CLHEP::RandFlat::shoot(0.0, 1.0); double ran1 = CLHEP::RandFlat::shoot(-1.0, 1.0); double ran2Pi = CLHEP::RandFlat::shoot(0.0, 2.0*CLHEP::pi); double t = CLHEP::RandFlat::shoot(100.0, 300.0);

double wl = CLHEP::RandFlat::shoot(4000.0, 6000.0); double r = pow(ran0, 1.0/3.0) * fPSUPRadius; // mm double costheta = ran1; double sintheta = sqrt(1.0 - costheta*costheta);

The MP Water Fitter uses prompt light and assumes that photons propagate in straight lines (straight light paths) for likelihood calculations. Detailed situations, such as the reflection and lensing effects from different detector components are neglected. Figure **??** shows the reconstruction concepts for position and direction.

The MPW fitter currently fits for position, time and direction of a water phase event. The fitter uses prompt light and straight line paths for likelihood calculations. Then it utilizes the Multi-path Fitter to maximize the likelihood functions and find the best-fit values. The concept of this fitter is the same of the FTU fitter in SNO time.

MPW: Fitter Structure The MPW fitter consists of:

- Fitter Data : Includes physics constants, set-values and pdfs for the MPW fitter. These parameters are set in the MPW database.

  - Water reflection index (water_RI, or n_{water}), used for group velocity (v_g =c/n_{water}) calculation.

  The MPW fitter currently uses one fixed number for n_{water}, rather than a function of wavelengths. The value of n_{water} can be tuned to give the lowest biases of the fitted positions to the Monte Carlo and to give the lowest RMS of fitted results as well. But the effect of n_{water} can also be corrected by the drive correction afterwards. Currently $n_{water} = 1.38486$ is obtained by analyzing the time of flight from the ^{16}N central run-100934 data reconstructed by the MPW fitter.

  - Constants for fit setting: Includes the fitter tolerance, the maximum iterations for the Multi-path Fitter to converge, time offset, radius cut for position vertex, fitting bin-width and steps.

- Other physics constants: air reflection index (air_RI), psup radius.

- PMT response time (timing) pdf for the position reconstruction, as shown in 4.1. The pdf shown in red line is modified from the measured PMT response time distribution from SNO time and the late light response is forced to be de-weighted (black). The pdf is modified in [-100,-4] ns region to match the time residue spectrum obtained from

Figure 3.1: PMT response time as the timing pdf.

- PMT angular response pdf for the direction reconstruction, as shown in 4.2. It is taken from the Monte Carlo simulation of 5 MeV electrons traverse in the AV with one direction.

Figure 3.2: PMT angular distribution as the angular response pdf.

- Fit the position, time and direction.

  - Likelihood Calculation Classes: Constructs likelihood functions, calculates likelihoods and their derivatives. For the MPW fitter, there are two classes: WaterPosition for position reconstruction and WaterDirection for direction reconstruction. The WaterPosition class tackles with 4 parameters (x,y,z,t) and the WaterDirection class tackles with 2 parameters (θ,ϕ).

  - Multi-path Fitter: Processes the MPW fitter and finds the best-fit of the likelihood function. It is a general processor and is shared with the fitters using the Multi-path Fitter, including the MPW fitter, air-water (AW) fitter, wavelength-shifter (WLS) fitter and scint-water fitter (being developed). It processes a certain fitter by being assigned the fitter name in macro. It processes the fitter event by event: for every triggered event, it first calls PMT selectors (ModeCut or StraightTimeResidualCut) and sends the information of the reduced PMTs to a certain Likelihood Calculation Class for likelihood calculations. The Likelihood Calculation Class sends back the values of likelihoods and their derivatives, so the Multi-path Fitter does not care about how the likelihood functions are constructed and how the likelihoods and derivatives are calculated. Using these values, it constructs an n×n Hessian matrix (n is the number of fitting parameters defined in Likelihood Calculation Class) and uses the Levenberg-Marquardt (MRQ) method to maximize the likelihood and finds the best-fit values. For the MPW, if the likelihood maxima is found 5 times for any position and direction then values are returned as the fitted position and direction. For the MPW case, it calls the ModeCut and fitsfor the position and time; then it calls the StraightTimeResidualCut and fits for the directions.

- Dump Likelihood: It is a function inside the Multi-path Fitter. It stores the likelihood surfaces and their derivatives from the fitting of the Multi-path Fitter to check whether the fitter finds global or local maximum of the interested events and to check the reconstruction performances. It requires a switch on/off parameter and the GTIDs of the interested events (a list of GTIDs) from the MPW database.

- SDecompQRH: It is a fit method class modified from ROOT TDecompQRH. It is used by the Multi-path Fitter to invert the Hessian matrix. Compared to ROOT, Solve() for Ax=b is modified to zero the component of x for which the diagonal element in R is small. This allows a Levenberg-Marquardt optimization to continue in many cases when the matrix is singular. For the MPW case, it is used to invert 4×4 matrix of the WaterPosition Class while the inversion of 2×2 matrix of the WaterDirection is calculated directly.

- ModeCut: The same class used by Rat. Selects the PMTs of an event by a mode time window. For the MPW, the optimized window is $[-50 + t_{mode}, 100 + t_{mode}]$ ns obtained from

- StraightTimeResidualCut: Selects the PMTs of an event by a time residue window. This selector requires a fitted position and fitted time. It calculates the time residue directly by assuming straight light path, which is the same method used by Multi-path fitter. For the MPW case, it is used for the direction fit after the position and time are reconstructed. The default window is [-10, 250] ns.

MPW: Position and Direction Reconstructions For the position reconstruction of the MPW fitter, the likelihood function simply calculates the likelihood assuming straight line paths of prompt light from a position vertex $\vec{X}_0$ (fVertex) and a starting time offset t_0 to each of the hit PMTs.

The time residue (t_{res}) is taken as the fitting parameter of the likelihood function for position reconstruction. The t_{res} of the i-th hit PMT is calculated as $t^i_{res} = t^i_{\text{pmt}} - |\vec{X}_0 - \vec{X}^i_{\text{pmt}}|/v_g - t_0$, where t^i_{pmt} is the hit time of the i-th hit PMT and $\vec{X}^i_{\text{pmt}}$ (fPosition) is the position of the i-th hit PMT. Then the likelihood function for position reconstruction is constructed as:

$$L(\vec{x}_0, t_0) = \sum_{i=1}^{\text{Nhits}} L_i(t^i_{res})$$

We define the position difference $\vec{X}_{\text{diffCh}} = \vec{X}_0 - \vec{X}_{\text{pmt}}$, then the time of flight for prompt light is $t_{\text{Ch}} = |\vec{X}_{\text{diffCh}}|/v_g$ and $L_{\text{Ch}} = L(t_{\text{Ch}})$.

The derivatives of the likelihood function can be calculated from explicit mathematical forms as:

$$\frac{\partial L}{\partial t_0} = \frac{dL_{\text{Ch}}}{dt_{\text{Ch}}},$$

$$\frac{\partial L}{\partial x} = \frac{\partial L_{\text{Ch}}}{\partial t_{\text{Ch}}}\frac{dt_{\text{Ch}}}{\partial x} = -\frac{dL_{\text{Ch}}}{dt_{\text{Ch}}}\frac{X_{\text{diffCh}}}{|\vec{X}_{\text{diffCh}}| \cdot v_g},$$

$$\frac{\partial L}{\partial y} = -\frac{dL_{\text{Ch}}}{dt_{\text{Ch}}}\frac{Y_{\text{diffCh}}}{|\vec{X}_{\text{diffCh}}| \cdot v_g},$$

$$\frac{\partial L}{\partial z} = -\frac{dL_{\text{Ch}}}{dt_{\text{Ch}}}\frac{Z_{\text{diffCh}}}{|\vec{X}_{\text{diffCh}}| \cdot v_g},$$

where $\frac{dL_{\text{Ch}}}{dt_{\text{Ch}}}$ can be calculated numerically from the timing pdf.

In the WaterPosition class, it starts with a random $(\vec{x}_0, t_0)$ as seed and calculates the likelihoods and their derivatives for various paths. These values are sent to the Multi-path Fitter, which is fitting 4 parameters: x, y, z, t and to maximize the likelihood function through the MRQ method and to find the best-fit positions.

For the direction reconstruction, the direction vertex $\vec{u}_0 = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)$ (fDirection), where the θ is zenith angle and ϕ the azimuth. $\cos\theta_{\text{Ch}}$ is the angle between $\vec{u}_0$ and $\vec{X}_{\text{diffCh}}$, which is taken as the fitting parameter of the likelihood function for the direction reconstruction. For the i-th hit PMT, $\cos\theta^i_{\text{Ch}} = \vec{u}_0 \cdot \frac{\vec{X}^i_{\text{diffCh}}}{|\vec{X}^i_{\text{diffCh}}|}$, then the likelihood function is:

$$L(\vec{u}_0) = \sum_{i=1}^{\text{Nhits}} L_i(\cos\theta^i_{\text{Ch}}),$$

The derivatives have explicit mathematical forms:

$$\frac{\partial L}{\partial\theta} = \frac{dL_{\text{Ch}}}{d\cos\theta_{\text{Ch}}}\frac{d\cos\theta_{\text{Ch}}}{\partial\theta} = \frac{dL_{\text{Ch}}}{d\cos\theta_{\text{Ch}}}\frac{d\vec{u}_0}{d\theta} \cdot \frac{\vec{X}_{\text{diffCh}}}{|\vec{X}_{\text{diffCh}}|},$$

where $d\vec{u}_0/d\theta = (\cos\phi\cos\theta, \sin\phi\cos\theta, -\sin\theta)$ and

$$\frac{\partial L}{\partial\phi} = \frac{dL_{\text{Ch}}}{d\cos\theta_{\text{Ch}}}\frac{d\cos\theta_{\text{Ch}}}{d\phi} = \frac{dL_{\text{Ch}}}{d\cos\theta_{\text{Ch}}}\frac{d\vec{u}_0}{d\phi} \cdot \frac{\vec{X}_{\text{diffCh}}}{|\vec{X}_{\text{diffCh}}|},$$

where $d\vec{u}_0/d\phi = (-\sin\phi\sin\theta, \cos\phi\sin\theta, 0)$. $\frac{dL_{\text{Ch}}}{d\cos\theta_{\text{Ch}}}$ can be calculated numerically from the PMT angular response pdf.

In the FitterWaterDirection class, it starts with a random (θ_0, ϕ_0) as seed and calculates the likelihoods and their derivatives for various paths. These values are sent to the Multi-path Fitter, which is now fitting 2 parameters: (θ, ϕ) and to maximize the likelihood function through the MRQ method and to find the best-fit directions.

MPW: Drive Correction Once the MPW fitter obtains the fitted position and direction, a drive correction is applied on the fitted position by $\vec{X}_{\text{corrected}} = p_0\vec{X}_{fit} + p_1\vec{u}_{fit}$, where p_0 and p_1 are the correction parameters.

To obtain the values of p_0 and p_1, we generated electron events distributed isotropically inside the AV. The simulations of 2, 3, 4, ... ,10 MeV electrons are produced. Then the MPW fitter is applied on each simulations and returns the results of $\vec{X}_{fit}$ and $\vec{u}_{fit}$. Take the Monte Carlo generated positions $\vec{X}_{MC}$ as the true positions, for all the fitted events, a

χ^2 function is calculated by:

$$\chi^2 = \sum_{i=1}^{N_{\text{events}}} [\vec{X}^i_{MC} - (p_0\vec{X}^i_{fit} + p_1\vec{u}^i_{fit})]^2$$

The p_0 and p_1 are obtained by minimizing the χ^2 function. When doing the χ^2 calculation, the fitted events of $|\vec{X}_{fit} - \vec{X}_{MC}| > 3\ m$ are thrown away to improve the χ^2 minimization results.

For the 2 to 10 MeV electrons simulations, the obtained values of p_0 and p_1 are energy or Nhit dependent. However, it does not improve the results if using the Nhit dependent functions $p_0(Nhit)$ and $p_1(Nhit)$ as drive corrections. Finally we take the average values from the 5 to 10 MeV electrons simulations and the drive correction is set as $\vec{X}_{\text{corrected}} = 0.995765\vec{X}_{fit} + -63.826\vec{u}_{fit}$.

It is important to note that since the drive correction parameters are obtained from the reconstructions of Monte Carlo, it depends on the Monte Carlo and the results of reconstruction. Therefore, the n_{water}, mode cut and time residue cut affecting the fitted results will also affect the drive correction parameters, but not significantly.

By fitting the simulations of 5 MeV electrons generated at the detector center and travelling along +X direction, the drive effct of the MPW fitter causes a ~50 mm biases from the detector center along +X axis. The drive correction reduces this drive bias down to ~0.2 mm. For the reconstruction of ^{16}N data, the drive correction can reduce the fitted position RMS by ~20 mm.

3.4 Likelihood Calculation

to fit the nonlinear model for multiple parameters, Levenberg-Marquardt method is used.

Taylor series expansion

$$\chi^2(\theta) \approx \chi^2(\theta_{current}) + \sum_k \frac{\partial \chi^2(\theta_{current})}{\partial \theta_k}\delta\theta_k + \frac{1}{2}\sum_{\alpha\beta} \frac{\partial^2 \chi^2(\theta_{current})}{\partial \theta_\alpha \theta_\beta}\delta\theta_\alpha\delta\theta_\beta$$

where

$$\kappa_{\alpha\beta} \equiv \frac{1}{2}\frac{\partial^2 \chi^2(\theta_{current})}{\partial \theta_\alpha \theta_\beta}$$

is defined as the curvature matrix[3].

3.5 ^{16}N test

emit γ-rays. These γ-rays will Compton scatter off electrons and the electrons will emit Cherenkov light to be detected by the PMTs.

3.6 Vertex Reconstruction for the SNO+ Partial-phase

For the partial-phase geometry, the SNO+ acrylic vessel can be considered as composed of the neck (cylinder), AV sphere and water-scintillator interface (plane). The ray coming from the vertex to the PMT can intersect with these three geometries.

line-sphere intersection and line-plane intersection

a_1, a_2 and a_3

trial position $\vec{X}_0 = (x_0, y_0, z_0)$, PMT position $\vec{X}_{\text{pmt}} = (x_{\text{pmt}}, y_{\text{pmt}}, z_{\text{pmt}})$

ray-vector $\vec{l_0} = \vec{X}_0 + a \cdot \vec{u}$, where a is the distance between vertex and intersection point. It is the parameter to be determined. $\vec{u} = (\vec{X}_{\text{pmt}} - \vec{X}_0)$ is the direction of the ray-vector/light path.

$\vec{O}_{av}$ is the origin of the AV sphere. In the PSUP coordinate, $\vec{O}_{av} = (0, 0, 108)\ mm$. For the ray-sphere intersection, $(\vec{l_0} - \vec{O}_{av})^2 = r_{av}^2$

To solve this equation, let $\Delta = [(\vec{X}_0 - \vec{O}_{av}) \cdot \vec{u}]^2 - (\vec{X}_0 - \vec{O}_{av})^2 + r_{av}^2$ then

$$a_{+,-} = -(\vec{X}_0 - \vec{O}_{av}) \cdot \vec{u} \pm \sqrt{\Delta},\ if \Delta > 0$$

if $\Delta \leq 0$, there is no intersection point or only one intersection point at the AV, the ray never passes through the AV sphere.

For the ray-plane intersection, $l_{0,z} = Z_{split}$, where Z_{split} is the water level. If $u_z = z_{\text{pmt}} - z_0 = 0$, the ray is parallel to the plane and never intersects the plane. To solve this equation, we have $a = (Z_{split} - z_0)/u_z = (Z_{split} - z_0),\ \ if\ u_z \neq 0$. Let:

$$a_3 \equiv a = \frac{(Z_{split} - z_0)|\vec{X}_{\text{pmt}} - \vec{X}_0|}{z_{\text{pmt}} - z_0}\ \ (if\ z_{\text{pmt}} - z_0 \neq 0),$$

For the ray-cylinder intersection, $l_{0,x}^2 + l_{0,y}^2 = r_{neck}^2$, where r_{neck} is the radius of the neck cylinder.

$$time\ of\ flight\ (tof) = (a_+ - a_3)/v_{gr,scint} + [|\vec{X}_{\mathrm{pmt}} - \vec{X}_0| - (a_+ - a_3)]/v_{gr,water}$$

$$\frac{\partial L}{\partial splitZ} = \frac{\partial L}{\partial tof} \cdot \frac{\partial tof}{\partial splitZ} = \frac{\partial L}{\partial tof} \cdot \frac{\partial a_3}{\partial splitZ}$$

$$\frac{\partial L}{\partial splitZ} = 0$$

scintillator timing

$$\sum_{i=1}^{i=4} a_i \cdot \frac{e^{-\frac{x}{t_i}} - e^{-\frac{x}{t_{rise}}}}{t_i - t_{rise}}$$

from bench top measurement, while the rise time, $t_{rise} = 0.8\ ns$ the timing parameters t_i, amplitude a_i are determined by the benchtop measurements

Table 3.1: scintillator α/β timing parameters**??**.

scintillator	timing [ns]				amplitudes			
particles	t_1	t_2	t_3	t_4	a_1	a_2	a_3	a_4
LAB + 2g/L PPO (default scintillator)								
e^-	4.88	15.4	66.0	400	0.665	0.218	0.083	0.0346
α	4.79	18.4	92.0	900	0.427	0.313	0.157	0.1027
LAB + 0.5g/L PPO (partial-fill phase)								
e^-	7.19	24.81	269.87	–	0.553	0.331	0.116	–
α	6.56	23.82	224.19	–	0.574	0.311	0.115	–
LAB + 2g/L PPO + 0.5% molar concentrations DDA								
e^-	5.0	12.1	33.3	499.0	0.68	0.21	0.07	0.04
α	3.8	11.3	65.3	758.0	0.48	0.32	0.14	0.06
LAB + 2g/L PPO + 0.5% molar concentrations Te+0.5% molar DDA								
e^-	3.7	10.0	52.0	500.0	0.72	0.23	0.02	0.03
α	3.69	15.5	79.3	489.0	0.63	0.23	0.07	0.07

timing spectrum

pdfs

Appendix: Levenberg-Marquardt method for fitter minimization (ref: press2007numerical)

for M unknown parameters: $a_0, a_1, ..., a_{M-1}$ (for example, the 4 parameters of an event vertex: (x, y, z, t))

the χ^2 function can be expanded and well approximated as

$$\chi^2(\mathbf{a}) \simeq \gamma - \mathbf{d} \cdot \mathbf{a} + \frac{1}{2}\mathbf{a} \cdot \mathbf{D} \cdot \mathbf{a},$$

$\mathbf{a}_{min} = \mathbf{a}_{cur} + \mathbf{D}^{-1} \cdot [-\nabla\chi^2(\mathbf{a}_{cur})]$

for a fudge factor λ,

$$\delta a_l = \frac{1}{\lambda\alpha_{ll}}\beta_l \ (\alpha_{ll} > 0),$$

$$\sum_{l=0}^{M-1} \alpha'_{kl}\delta a_l = \beta_k$$

Let $\alpha \equiv \frac{1}{2}\mathbf{D}$, which is the half Hessian, or called as curvature matrix.

$\beta_k = -\frac{1}{2}\frac{\partial\chi^2}{\partial a_k},\ \alpha_{kl} = \frac{1}{2}\frac{\partial^2\chi^2}{\partial a_k \partial a_l}$

by optimizations, the values of tolerance, are set to .

Chapter 4

Partial-filled Scintillator Phase

.q

4.1 Reconstruction of the SNO+

4.2 Reconstruction Algorithms for Position, Time and Energy of Events in SNO+

4.3 An Alternative Vertex Reconstruction Algorithm for SNO+

A Multi-path Fitter (MPF) framework was developed by the University of Alberta group as an alternative reconstruction algorithm to the SNO+ official fitter. In this framework, fitters for SNO+ water phase (MP Water Fitter), wavelength shifter (MP WLS Fitter), partial-fill phase (MP Partial Fitter) and scintillator phase (MP Scint Fitter) were developed. In SNO+ water phase, the cavity and the AV are both filled with pure water. This is a relatively simple geometry. Therefore, we start with the MP Water Fitter to explain the reconstruction concepts.

First, the fitter throws a random vertex (uniformly distributing) inside the PSUP as a trial vertex. The Class Library for High Energy Physics (CLHEP) is used for creating pseudo-random numbers.

$rand0 = Uniform(0,1), rand1 = Uniform(-1,1)$

double ran0 = CLHEP::RandFlat::shoot(0.0, 1.0); double ran1 = CLHEP::RandFlat::shoot(-1.0, 1.0); double ran2Pi = CLHEP::RandFlat::shoot(0.0, 2.0*CLHEP::pi); double t = CLHEP::RandFlat::shoot(100.0, 300.0);

double wl = CLHEP::RandFlat::shoot(4000.0, 6000.0); double r = pow(ran0, 1.0/3.0) * fPSUPRadius; // mm double costheta = ran1; double sintheta = sqrt(1.0 - costheta*costheta);

The MP Water Fitter uses prompt light and assumes that photons propagate in straight lines (straight light paths) for likelihood calculations. Detailed situations, such as the reflection and lensing effects from different detector components are neglected. Figure **??** shows the reconstruction concepts for position and direction.

The MPW fitter currently fits for position, time and direction of a water phase event. The fitter uses prompt light and straight line paths for likelihood calculations. Then it utilizes the Multi-path Fitter to maximize the likelihood functions and find the best-fit values. The concept of this fitter is the same of the FTU fitter in SNO time.

MPW: Fitter Structure The MPW fitter consists of:

- Fitter Data : Includes physics constants, set-values and pdfs for the MPW fitter. These parameters are set in the MPW database.

  - Water reflection index (water_RI, or n_{water}), used for group velocity (v_g =c/n_{water}) calculation.

  The MPW fitter currently uses one fixed number for n_{water}, rather than a function of wavelengths. The value of n_{water} can be tuned to give the lowest biases of the fitted positions to the Monte Carlo and to give the lowest RMS of fitted results as well. But the effect of n_{water} can also be corrected by the drive correction afterwards. Currently n_{water} = 1.38486 is obtained by analyzing the time of flight from the ^{16}N central run-100934 data reconstructed by the MPW fitter.

  - Constants for fit setting: Includes the fitter tolerance, the maximum iterations for the Multi-path Fitter to converge, time offset, radius cut for position vertex, fitting bin-width and steps.

- Other physics constants: air reflection index (air_RI), psup radius.

- PMT response time (timing) pdf for the position reconstruction, as shown in 4.1. The pdf shown in red line is modified from the measured PMT response time distribution from SNO time and the late light response is forced to be de-weighted (black). The pdf is modified in [-100,-4] ns region to match the time residue spectrum obtained from

Figure 4.1: PMT response time as the timing pdf.

- PMT angular response pdf for the direction reconstruction, as shown in 4.2. It is taken from the Monte Carlo simulation of 5 MeV electrons traverse in the AV with one direction.

Figure 4.2: PMT angular distribution as the angular response pdf.

- Fit the position, time and direction.

  - Likelihood Calculation Classes: Constructs likelihood functions, calculates likelihoods and their derivatives. For the MPW fitter, there are two classes: WaterPosition for position reconstruction and WaterDirection for direction reconstruction. The WaterPosition class tackles with 4 parameters (x,y,z,t) and the WaterDirection class tackles with 2 parameters (θ,ϕ).

  - Multi-path Fitter: Processes the MPW fitter and finds the best-fit of the likelihood function. It is a general processor and is shared with the fitters using the Multi-path Fitter, including the MPW fitter, air-water (AW) fitter, wavelength-shifter (WLS) fitter and scint-water fitter (being developed). It processes a certain fitter by being assigned the fitter name in macro. It processes the fitter event by event: for every triggered event, it first calls PMT selectors (ModeCut or StraightTimeResidualCut) and sends the information of the reduced PMTs to a certain Likelihood Calculation Class for likelihood calculations. The Likelihood Calculation Class sends back the values of likelihoods and their derivatives, so the Multi-path Fitter does not care about how the likelihood functions are constructed and how the likelihoods and derivatives are calculated. Using these values, it constructs an n×n Hessian matrix (n is the number of fitting parameters defined in Likelihood Calculation Class) and uses the Levenberg-Marquardt (MRQ) method to maximize the likelihood and finds the best-fit values. For the MPW, if the likelihood maxima is found 5 times for any position and direction then values are returned as the fitted position and direction. For the MPW case, it calls the ModeCut and fitsfor the position and time; then it calls the StraightTimeResidualCut and fits for the directions.

- Dump Likelihood: It is a function inside the Multi-path Fitter. It stores the likelihood surfaces and their derivatives from the fitting of the Multi-path Fitter to check whether the fitter finds global or local maximum of the interested events and to check the reconstruction performances. It requires a switch on/off parameter and the GTIDs of the interested events (a list of GTIDs) from the MPW database.

- SDecompQRH: It is a fit method class modified from ROOT TDecompQRH. It is used by the Multi-path Fitter to invert the Hessian matrix. Compared to ROOT, Solve() for Ax=b is modified to zero the component of x for which the diagonal element in R is small. This allows a Levenberg-Marquardt optimization to continue in many cases when the matrix is singular. For the MPW case, it is used to invert 4×4 matrix of the WaterPosition Class while the inversion of 2×2 matrix of the WaterDirection is calculated directly.

- ModeCut: The same class used by Rat. Selects the PMTs of an event by a mode time window. For the MPW, the optimized window is $[-50 + t_{mode}, 100 + t_{mode}]$ ns obtained from

- StraightTimeResidualCut: Selects the PMTs of an event by a time residue window. This selector requires a fitted position and fitted time. It calculates the time residue directly by assuming straight light path, which is the same method used by Multi-path fitter. For the MPW case, it is used for the direction fit after the position and time are reconstructed. The default window is [-10, 250] ns.

MPW: Position and Direction Reconstructions For the position reconstruction of the MPW fitter, the likelihood function simply calculates the likelihood assuming straight line paths of prompt light from a position vertex $\vec{X}_0$ (fVertex) and a starting time offset t_0 to each of the hit PMTs.

The time residue (t_{res}) is taken as the fitting parameter of the likelihood function for position reconstruction. The t_{res} of the i-th hit PMT is calculated as $t^i_{res} = t^i_{\text{pmt}} - |\vec{X}_0 - \vec{X}^i_{\text{pmt}}|/v_g - t_0$, where t^i_{pmt} is the hit time of the i-th hit PMT and $\vec{X}^i_{\text{pmt}}$ (fPosition) is the position of the i-th hit PMT. Then the likelihood function for position reconstruction is constructed as:

$$L(\vec{x}_0, t_0) = \sum_{i=1}^{\text{Nhits}} L_i(t^i_{res})$$

We define the position difference $\vec{X}_{\text{diffCh}} = \vec{X}_0 - \vec{X}_{\text{pmt}}$, then the time of flight for prompt light is $t_{\text{Ch}} = |\vec{X}_{\text{diffCh}}|/v_g$ and $L_{\text{Ch}} = L(t_{\text{Ch}})$.

The derivatives of the likelihood function can be calculated from explicit mathematical forms as:

$$\frac{\partial L}{\partial t_0} = \frac{dL_{\text{Ch}}}{dt_{\text{Ch}}},$$

$$\frac{\partial L}{\partial x} = \frac{\partial L_{\text{Ch}}}{\partial t_{\text{Ch}}} \frac{dt_{\text{Ch}}}{\partial x} = -\frac{dL_{\text{Ch}}}{dt_{\text{Ch}}} \frac{X_{\text{diffCh}}}{|\vec{X}_{\text{diffCh}}| \cdot v_g},$$

$$\frac{\partial L}{\partial y} = -\frac{dL_{\text{Ch}}}{dt_{\text{Ch}}} \frac{Y_{\text{diffCh}}}{|\vec{X}_{\text{diffCh}}| \cdot v_g},$$

$$\frac{\partial L}{\partial z} = -\frac{dL_{\text{Ch}}}{dt_{\text{Ch}}} \frac{Z_{\text{diffCh}}}{|\vec{X}_{\text{diffCh}}| \cdot v_g},$$

where $\frac{dL_{\text{Ch}}}{dt_{\text{Ch}}}$ can be calculated numerically from the timing pdf.

In the WaterPosition class, it starts with a random $(\vec{x}_0, t_0)$ as seed and calculates the likelihoods and their derivatives for various paths. These values are sent to the Multi-path Fitter, which is fitting 4 parameters: x, y, z, t and to maximize the likelihood function through the MRQ method and to find the best-fit positions.

For the direction reconstruction, the direction vertex $\vec{u}_0 = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)$ (fDirection), where the θ is zenith angle and ϕ the azimuth. $\cos\theta_{\mathrm{Ch}}$ is the angle between $\vec{u}_0$ and $\vec{X}_{\mathrm{diffCh}}$, which is taken as the fitting parameter of the likelihood function for the direction reconstruction. For the i-th hit PMT, $\cos\theta^i_{\mathrm{Ch}} = \vec{u}_0 \cdot \frac{\vec{X}^i_{\mathrm{diffCh}}}{|\vec{X}^i_{\mathrm{diffCh}}|}$, then the likelihood function is:

$$L(\vec{u}_0) = \sum_{i=1}^{\mathrm{Nhits}} L_i(\cos\theta^i_{\mathrm{Ch}}),$$

The derivatives have explicit mathematical forms:

$$\frac{\partial L}{\partial\theta} = \frac{dL_{\mathrm{Ch}}}{d\cos\theta_{\mathrm{Ch}}}\frac{d\cos\theta_{\mathrm{Ch}}}{\partial\theta} = \frac{dL_{\mathrm{Ch}}}{d\cos\theta_{\mathrm{Ch}}}\frac{d\vec{u}_0}{d\theta} \cdot \frac{\vec{X}_{\mathrm{diffCh}}}{|\vec{X}_{\mathrm{diffCh}}|},$$

where $d\vec{u}_0/d\theta = (\cos\phi\cos\theta, \sin\phi\cos\theta, -\sin\theta)$ and

$$\frac{\partial L}{\partial\phi} = \frac{dL_{\mathrm{Ch}}}{d\cos\theta_{\mathrm{Ch}}}\frac{d\cos\theta_{\mathrm{Ch}}}{d\phi} = \frac{dL_{\mathrm{Ch}}}{d\cos\theta_{\mathrm{Ch}}}\frac{d\vec{u}_0}{d\phi} \cdot \frac{\vec{X}_{\mathrm{diffCh}}}{|\vec{X}_{\mathrm{diffCh}}|},$$

where $d\vec{u}_0/d\phi = (-\sin\phi\sin\theta, \cos\phi\sin\theta, 0)$. $\frac{dL_{\mathrm{Ch}}}{d\cos\theta_{\mathrm{Ch}}}$ can be calculated numerically from the PMT angular response pdf.

In the FitterWaterDirection class, it starts with a random (θ_0, ϕ_0) as seed and calculates the likelihoods and their derivatives for various paths. These values are sent to the Multi-path Fitter, which is now fitting 2 parameters: (θ, ϕ) and to maximize the likelihood function through the MRQ method and to find the best-fit directions.

MPW: Drive Correction Once the MPW fitter obtains the fitted position and direction, a drive correction is applied on the fitted position by $\vec{X}_{\mathrm{corrected}} = p_0\vec{X}_{fit} + p_1\vec{u}_{fit}$, where p_0 and p_1 are the correction parameters.

To obtain the values of p_0 and p_1, we generated electron events distributed isotropically inside the AV. The simulations of 2, 3, 4, ... ,10 MeV electrons are produced. Then the MPW fitter is applied on each simulations and returns the results of $\vec{X}_{fit}$ and $\vec{u}_{fit}$. Take the Monte Carlo generated positions $\vec{X}_{MC}$ as the true positions, for all the fitted events, a

χ^2 function is calculated by:

$$\chi^2 = \sum_{i=1}^{N_{\text{events}}} [\vec{X}^i_{MC} - (p_0\vec{X}^i_{fit} + p_1\vec{u}^i_{fit})]^2$$

The p_0 and p_1 are obtained by minimizing the χ^2 function. When doing the χ^2 calculation, the fitted events of $|\vec{X}_{fit} - \vec{X}_{MC}| > 3\ m$ are thrown away to improve the χ^2 minimization results.

For the 2 to 10 MeV electrons simulations, the obtained values of p_0 and p_1 are energy or Nhit dependent. However, it does not improve the results if using the Nhit dependent functions $p_0(Nhit)$ and $p_1(Nhit)$ as drive corrections. Finally we take the average values from the 5 to 10 MeV electrons simulations and the drive correction is set as $\vec{X}_{\text{corrected}} = 0.995765\vec{X}_{fit} + -63.826\vec{u}_{fit}$.

It is important to note that since the drive correction parameters are obtained from the reconstructions of Monte Carlo, it depends on the Monte Carlo and the results of reconstruction. Therefore, the n_{water}, mode cut and time residue cut affecting the fitted results will also affect the drive correction parameters, but not significantly.

By fitting the simulations of 5 MeV electrons generated at the detector center and travelling along +X direction, the drive effct of the MPW fitter causes a ∼50 mm biases from the detector center along +X axis. The drive correction reduces this drive bias down to ∼0.2 mm. For the reconstruction of ^{16}N data, the drive correction can reduce the fitted position RMS by ∼20 mm.

4.4 Likelihood Calculation

to fit the nonlinear model for multiple parameters, Levenberg-Marquardt method is used.

Taylor series expansion

$$\chi^2(\theta) \approx \chi^2(\theta_{current}) + \sum_k \frac{\partial\chi^2(\theta_{current})}{\partial\theta_k}\delta\theta_k + \frac{1}{2}\sum_{\alpha\beta}\frac{\partial^2\chi^2(\theta_{current})}{\partial\theta_\alpha\theta_\beta}\delta\theta_\alpha\delta\theta_\beta$$

where

$$\kappa_{\alpha\beta} \equiv \frac{1}{2}\frac{\partial^2\chi^2(\theta_{current})}{\partial\theta_\alpha\theta_\beta}$$

is defined as the curvature matrix[3].

4.5 ^{16}N test

emit γ-rays. These γ-rays will Compton scatter off electrons and the electrons will emit Cherenkov light to be detected by the PMTs.

4.6 Vertex Reconstruction for the SNO+ Partial-phase

For the partial-phase geometry, the SNO+ acrylic vessel can be considered as composed of the neck (cylinder), AV sphere and water-scintillator interface (plane). The ray coming from the vertex to the PMT can intersect with these three geometries.

line-sphere intersection and line-plane intersection

a_1, a_2 and a_3

trial position $\vec{X}_0 = (x_0, y_0, z_0)$, PMT position $\vec{X}_{\text{pmt}} = (x_{\text{pmt}}, y_{\text{pmt}}, z_{\text{pmt}})$

ray-vector $\vec{l}_0 = \vec{X}_0 + a \cdot \vec{u}$, where a is the distance between vertex and intersection point. It is the parameter to be determined. $\vec{u} = (\vec{X}_{\text{pmt}} - \vec{X}_0)$ is the direction of the ray-vector/light path.

$\vec{O}_{av}$ is the origin of the AV sphere. In the PSUP coordinate, $\vec{O}_{av} = (0, 0, 108)\ mm$. For the ray-sphere intersection, $(\vec{l}_0 - \vec{O}_{av})^2 = r_{av}^2$

To solve this equation, let $\Delta = [(\vec{X}_0 - \vec{O}_{av}) \cdot \vec{u}]^2 - (\vec{X}_0 - \vec{O}_{av})^2 + r_{av}^2$ then

$$a_{+,-} = -(\vec{X}_0 - \vec{O}_{av}) \cdot \vec{u} \pm \sqrt{\Delta},\ if \Delta > 0$$

if $\Delta \leq 0$, there is no intersection point or only one intersection point at the AV, the ray never passes through the AV sphere.

For the ray-plane intersection, $l_{0,z} = Z_{split}$, where Z_{split} is the water level. If $u_z = z_{\text{pmt}} - z_0 = 0$, the ray is parallel to the plane and never intersects the plane. To solve this equation, we have $a = (Z_{split} - z_0)/u_z = (Z_{split} - z_0),\ \ if\ u_z \neq 0$. Let:

$$a_3 \equiv a = \frac{(Z_{split} - z_0)|\vec{X}_{\text{pmt}} - \vec{X}_0|}{z_{\text{pmt}} - z_0}\ \ (if\ z_{\text{pmt}} - z_0 \neq 0),$$

For the ray-cylinder intersection, $l_{0,x}^2 + l_{0,y}^2 = r_{neck}^2$, where r_{neck} is the radius of the neck cylinder.

$$time\ of\ flight\ (tof) = (a_+ - a_3)/v_{gr,scint} + [|\vec{X}_{\mathrm{pmt}} - \vec{X}_0| - (a_+ - a_3)]/v_{gr,water}$$

$$\frac{\partial L}{\partial splitZ} = \frac{\partial L}{\partial tof} \cdot \frac{\partial tof}{\partial splitZ} = \frac{\partial L}{\partial tof} \cdot \frac{\partial a_3}{\partial splitZ}$$

$$\frac{\partial L}{\partial splitZ} = 0$$

scintillator timing

$$\sum_{i=1}^{i=4} a_i \cdot \frac{e^{-\frac{x}{t_i}} - e^{-\frac{x}{t_{rise}}}}{t_i - t_{rise}}$$

from bench top measurement, while the rise time, $t_{rise} = 0.8\ ns$ the timing parameters t_i, amplitude a_i are determined by the benchtop measurements

Table 4.1: scintillator α/β timing parameters**??**.

scintillator	timing [ns]				amplitudes			
particles	t_1	t_2	t_3	t_4	a_1	a_2	a_3	a_4
LAB + 2g/L PPO (default scintillator)								
e^-	4.88	15.4	66.0	400	0.665	0.218	0.083	0.0346
α	4.79	18.4	92.0	900	0.427	0.313	0.157	0.1027
LAB + 0.5g/L PPO (partial-fill phase)								
e^-	7.19	24.81	269.87	–	0.553	0.331	0.116	–
α	6.56	23.82	224.19	–	0.574	0.311	0.115	–
LAB + 2g/L PPO + 0.5% molar concentrations DDA								
e^-	5.0	12.1	33.3	499.0	0.68	0.21	0.07	0.04
α	3.8	11.3	65.3	758.0	0.48	0.32	0.14	0.06
LAB + 2g/L PPO + 0.5% molar concentrations Te+0.5% molar DDA								
e^-	3.7	10.0	52.0	500.0	0.72	0.23	0.02	0.03
α	3.69	15.5	79.3	489.0	0.63	0.23	0.07	0.07

timing spectrum

pdfs

Appendix: Levenberg-Marquardt method for fitter minimization (ref: press2007numerical)

for M unknown parameters: $a_0, a_1, ..., a_{M-1}$ (for example, the 4 parameters of an event vertex: (x, y, z, t))

the χ^2 function can be expanded and well approximated as

$$\chi^2(\mathbf{a}) \simeq \gamma - \mathbf{d} \cdot \mathbf{a} + \frac{1}{2}\mathbf{a} \cdot \mathbf{D} \cdot \mathbf{a},$$

$\mathbf{a}_{min} = \mathbf{a}_{cur} + \mathbf{D}^{-1} \cdot [-\nabla\chi^2(\mathbf{a}_{cur})]$

for a fudge factor λ,

$$\delta a_l = \frac{1}{\lambda\alpha_{ll}}\beta_l \ (\alpha_{ll} > 0),$$

$$\sum_{l=0}^{M-1} \alpha'_{kl}\delta a_l = \beta_k$$

Let $\alpha \equiv \frac{1}{2}\mathbf{D}$, which is the half Hessian, or called as curvature matrix.

$\beta_k = -\frac{1}{2}\frac{\partial\chi^2}{\partial a_k}, \ \alpha_{kl} = \frac{1}{2}\frac{\partial^2\chi^2}{\partial a_k \partial a_l}$

by optimizations, the values of tolerance, are set to .

Appendix A

Appendix Name

References

[1] Muons. `https://cosmic.lbl.gov/SKliewer/Cosmic_Rays/Muons.htm`, 2001. [Online; accessed 19-July-2019].

[2] M. Agostini, A. Bakalyarov, M. Balata, I. Barabanov, L. Baudis, C. Bauer, E. Bellotti, S. Belogurov, A. Bettini, L. Bezrukov, et al. Probing majorana neutrinos with double-β decay. *Science*, page eaav8613, 2019.

[3] P. Gregory. *Bayesian Logical Data Analysis for the Physical Sciences: A Comparative Approach with Mathematica® Support*. Cambridge University Press, 2005.

[4] J. Paton. Neutrinoless Double Beta Decay in the SNO+ Experiment. In *Prospects in Neutrino Physics (NuPhys2018) London, United Kingdom, December 19-21, 2018*, 2019.

[5] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. *Numerical recipes 3rd edition: The art of scientific computing*. Cambridge university press, 2007.