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Measuring θ_{12} despite an uncertain reactor neutrino spectrum

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Abstract

The recently discovered 5-7 MeV excess in the reactor neutrino spectral structure, corresponding to a prompt energy of 4-6 MeV, highlights that the uncertainty in the reactor neutrino spectrum is far greater than some theoretical estimates. Medium baseline (about 50 km) reactor neutrino experiments will deliver by far the most precise ever measurements of θ_{12} . However, the theoretical reactor neutrino spectra, as they were recalculated in 2011, do not reproduce this excess. As a result, if a medium baseline experiment attempted to determine $\sin^2(2\theta_{12})$ using the theoretical spectrum, the result would have a systematic upward bias of 1%, much larger than the expected uncertainty. We show that by using recent measurements of the reactor neutrino spectrum the precision of a measurement of θ_{12} at a medium baseline reactor neutrino experiment can be improved appreciably. We estimate this precision as a function of the ⁹Li spallation background veto efficiency and dead time.

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1. Introduction

In about 5 years the largest liquid scintillator detectors ever built will be used to detect reactor neutrinos at the experiments JUNO [1] and RENO 50 [2]. The often-stated goal of these experiments is the determination of the neutrino mass hierarchy, following the strategy of Petcov and Piai [3]. Obtaining the required precision for a determination of the hierarchy will be very challenging [4–7]. On the other hand, whether or not this precision can be achieved, there is no doubt that such experiments can provide by far the most precise measurement yet of θ_{12} [8].

In this note we will show that imperfect knowledge of the shape of the reactor neutrino spectrum is a leading source of uncertainty in the measurement of θ_{12} and that this uncertainty has been systematically underestimated in the literature [9,10]. Studies of this measurement use the latest reactor neutrino flux model from Ref. [11], as improved in Ref. [12] with the inclusion of several additional effects. They also use the uncertainties quoted in that paper. Nonetheless, as the author clearly stated in Ref. [13], the uncertainty quoted in Ref. [12] reflects only a subset of the sources of uncertainty in the analysis and so in fact yields only a lower bound on the true uncertainty. As described in [13], without individually analyzing all of the decay chains, it is difficult even to determine how large the total uncertainty should be or what might provide the largest contributions.

One proposal for a source of the excess, and so the uncertainty in the original calculation, has been presented in Ref. [14]. In Ref. [15] the authors study ⁹²Rb decays, which provide large contributions to reactor spectra in the energy range of the excess. They find a ground state to ground state feeding that is in strong disagreement with standard value of Ref. [16], which was used in Ref. [14], but would itself lead to an excess of the observed form. In either case, the reactor anomaly of Ref. [17] appears to reflect a systematic underestimation of the uncertainty in estimates of reactor neutrino fluxes.

Our analysis will yield its own estimate of the expected uncertainty in θ_{12} . While this estimate is necessarily quite precise, it will not be accurate. An accurate determination would require the full covariance matrix of uncertainties for the spectrum generated by each isotope 10 years from now, when the data from these experiments is analyzed. However such a covariance matrix or isotope by isotope analysis is not available even now. Of course a *theoretical* covariance matrix was already proposed in Refs. [11,12] and used in the analysis of Ref. [10]. However, as was described above, those uncertainties appear to have been underestimated and indeed are quite challenging to estimate, and so JUNO will instead use a covariance matrix which is determined experimentally.

Our motivation for writing this paper now, when an experimentally determined covariance matrix for the uncertainties is not yet available, is as follows. In a companion paper [18] we consider the tracking requirements for cosmogenic muons for such experiments. For this, we need to know not the absolute value of the uncertainty in θ_{12} , but rather its expected dependence on the background rejection efficiency. While the absolute value of the uncertainty that we will obtain is quite approximate, the current paper nonetheless demonstrates that the uncertainty in θ_{12} receives a large contribution from systematic errors. This means that little is lost by increasing the statistical fluctuations via a veto strategy with a large dead time. In Ref. [18] we demonstrate that, as a consequence, a very high spallation background rejection efficiency is optimal for the θ_{12} measurement, higher than that for the mass hierarchy. This result is quite robust.

2. The theoretical uncertainty has been underestimated

2.1. Spallation isotope background

In all of the calculations that follow we will consider the ⁹Li spallation isotope background expected at JUNO. This is about 60% greater than that expected at RENO 50, and so our results may be easily adapted to RENO 50 by simply increasing the rejection efficiency without increasing the dead time. The spallation isotope rates were calculated in Ref. [19]. For completeness, we will summarize that calculation here.

We began with the parametrization of Ref. [20] for the muon flux as a function of energy, angle and depth in water. We converted the water depth to a rock depth. As the JUNO and RENO 50 experiments will be located under mountains, the depth is not uniform but rather depends on the direction from which the muon arrives. We used maps of the sites to parametrize this dependence. Then we used FLUKA [21] to model the propagation of muons in a spherical tank filled with 20 ktons of the scintillator LAB, corresponding to the JUNO detector. We found the rates of production of the isotopes ⁹Li and ⁸He from interactions of the muons with ¹²C in the scintillator. We multiplied these rates by the probability that their decay includes a neutron and so yields a false double coincidence. This product is our total background rate.

As the ⁸He rate is smaller than the ⁹Li rate by a factor of 30, in the present study we have simply ignored it. In this paper we have also included an 8.5 MeV maximum energy veto, which has little effect on the signal but further reduces the ⁹Li background by 28%. The background is included in all results below. However, to read the result with no background from our main results, summarized in Fig. 2 below, one need only consider the bottom curve, corresponding to no dead time, and the right end of the curve, corresponding to a perfect rejection efficiency.

2.2. Effect of the bump on θ_{12}

In this subsection we will motivate our new analysis of the precision of a measurement of θ_{12} by showing that the uncertainty in the theoretical spectrum [11,12], which has been used in previous determinations of the precision, was greatly underestimated. Our new study, which will be the subject of Sec. 3, will therefore provide a somewhat more reliable determination of this precision.

Recently a 5 MeV bump in the ratio of the measured reactor neutrino spectrum to the theoretical spectrum of [12] has been observed by RENO [22,23], Double Chooz [24] and Daya Bay [25]. As can be seen for example in Fig. 5 of Ref. [25] or Fig. 6 of Ref. [23], the amplitude of this bump is more than 10%, corresponding to a measured spectrum which, at prompt energies of 4–6 MeV exceeds the theoretical spectrum by 4σ in terms of the theoretical reactor flux uncertainties of Ref. [12]. Therefore it is clear that the difference between the true reactor spectrum and that of Ref. [12] is appreciably larger than the subset of the uncertainties which were quantified in that work.

To reassess the validity of a determination of the precision of a measurement of θ_{12} based on the theoretical spectrum, we will now answer the following question: What effect does the bump have on a determination of θ_{12} ?

Let us fix the neutrino mass splittings to be

$$\Delta M_{31}^2 = 2.4 \times 10^{-3} \text{ eV}^2 \qquad \Delta M_{21}^2 = 7.5 \times 10^{-5} \text{ eV}^2 \tag{2.1}$$



Fig. 1. From top to bottom at 5 MeV the curves are the inverse β decay event spectrum without oscillations, with oscillations and the ⁹Li event spectrum.

with the normal mass hierarchy and the relevant neutrino mixing angles to be

$$\sin^2(2\theta_{13}) = 0.089, \ \sin^2(2\theta_{12}) = 0.857.$$
(2.2)

We normalize the $\bar{\nu}_e$ flux at JUNO by setting the number of IBD events to be 10^5 for a 6 year run at a baseline of 58 km, but we adapt the correct baselines from Ref. [1]; we expect 1.3×10^5 IBD events in 6 years.

The only background that we consider is cosmogenic ⁹Li with the rate given in Ref. [19]. Using a cut at 8.5 MeV, we found that the expected number of background events is 8.3×10^4 in 6 years, of the same order of magnitude as the signal. In Fig. 1 we plot the reactor neutrino spectrum with and without the oscillations and the background spectrum. In practice most of this background can be vetoed and below we perform our analysis for various values of the veto efficiency.

For the calculation of χ^2 , in addition to θ_{12} , we minimize three pull parameters corresponding to the flux normalization of the spectrum and background, with uncertainties of 5% and 1% respectively, and also the value $\sin^2(2\theta_{13})$ with an uncertainty of 0.01. The background uncertainty corresponds to the expected statistical fluctuations in the background events, whereas the signal uncertainty was chosen somewhat arbitrarily to correspond to the size of the reactor anomaly in Ref. [17]. Variations of the later two uncertainties have little effect on our results. We divided the energy spectrum in region between 1.5 and 8.5 MeV into 233 30-keV bins. This information is assembled into our χ^2 function

$$\chi^{2}(\theta_{12}^{fit}, \alpha, \beta, \theta_{13}^{fit}) = \sum_{i=1}^{233} \frac{(N_{i}(\theta_{12}, \theta_{13}) + N_{i}^{back} - (1+\alpha)N_{i}(\theta_{12}^{fit}, \theta_{13}^{fit}) - (1+\beta)N_{i}^{back})^{2}}{N_{i}(\theta_{12}, \theta_{13}) + N_{i}^{back}} + \frac{\alpha^{2}}{\sigma_{\alpha}^{2}} + \frac{\beta^{2}}{\sigma_{\beta}^{2}} + \frac{(\sin^{2}(2\theta_{13}) - \sin^{2}(2\theta_{13}^{fit}))^{2}}{\sigma_{13}^{2}}$$
(2.3)

which we minimize with respect to the pull parameters α , β and θ_{13}^{fit} corresponding the signal and background normalizations and $\sin^2(2\theta_{13})$, which have uncertainties of σ_{α} , σ_{β} and σ_{13} respectively. Here $N_i(\theta_{12}, \theta_{13})$ and N_i^{back} are the expected number of reactor neutrino and background events in the bin *i*, and the values of θ_{13} and θ_{12} are given in Eq. (2.2).

Assuming a perfectly understood nonlinear energy response for the detector, we find that if the true reactor spectrum is that observed by Daya Bay in Ref. [25] but it is fit to the theoretical spectrum of Ref. [12] then the lowest χ^2 fit would arise with a value of $\sin^2(2\theta_{12})$ which is

more than 0.01 greater than the true value for all values of the background rejection efficiency, including the case with no backgrounds. This is because the excess in the measured spectrum leads to relatively less events at the solar oscillation maximum, around 3 MeV, and more events at higher energies, away from the maximum. A higher value of $\sin^2(2\theta_{12})$ also reduces the number of events at the solar maximum relative to other energies, and so an unexpected 5 MeV excess leads to a positive systematic bias in the fit value of $\sin^2(2\theta_{12})$.

By comparison, studies in the literature on the precision of a measurement of $\sin^2(2\theta_{12})$ using the uncertainty reported in Ref. [12] estimate a precision of, for example, 0.3% including the uncertainty caused by a model of the detector's nonlinear energy response [10]. Thus, were θ_{12} determined using the theoretical model [12] of the reactor spectra then the value obtained would differ from the true value by four times the uncertainty reported in, for instance, Ref. [10].

One might object that it is obvious that, now that the bump has been discovered, one should use the spectrum with the bump for all analyses. This is of course true. However it means that a new analysis is needed of the precision with which θ_{12} can be determined. This is the goal of the present paper.

3. The uncertainty with which θ_{12} may be measured

In this section we will determine the uncertainty with which θ_{12} may be measured at JUNO or RENO 50. Our strategy will be as follows. First in Subsec. 3.1 we will determine the uncertainty in θ_{12} resulting from the uncertainty in the reactor spectrum *measured* by Daya Bay. This differs from the approach in the previous section because we use the uncertainty in a measurement, not in a theoretical calculation. We estimate this uncertainty simply by finding the size of a shift in θ_{12} which can be compensated by a shift in the reactor spectrum which differs from Daya Bay's best fit reactor spectrum by precisely 1σ . Then in Subsec. 3.2 we will assume that the reactor spectrum is perfectly understood and calculate the uncertainty expected in θ_{12} from all other sources, such as statistical fluctuations and uncertainties in the various flux normalizations, etc. This analysis is similar to that in Ref. [9]. Finally, in Subsec. 3.3, we will obtain a rough estimate of the total uncertainty expected in θ_{12} by adding the contributions from the previous two subsections in quadrature.

3.1. Effect of the reactor spectrum uncertainty

In this note we would like to observe that the precise measurements of the reactor spectrum by the Daya Bay [25] and at the RENO near detector [23] in fact allow for a precise determination of θ_{12} . An accurate determination of the uncertainty which may be expected in θ_{12} would require, for each isotope, a covariance matrix of the errors in Refs. [25]. Such a set of covariance matrices has not yet been experimentally determined. So we simply sum in quadrature the bin per bin statistical and systematic errors reported by Daya Bay and treat them as uncorrelated.

As the entire spectrum, as measured at JUNO or RENO 50, corresponds to only half of a 1–2 flavor oscillation, only broad features of the spectrum will be important for measuring θ_{12} . Therefore even if the underlying reactor spectrum has a rich structure at scales of order 200 keV or smaller, which was not observed in Ref. [25] due to binning and the finite energy resolution, this will have no effect on the determination of θ_{12} . On the other hand the determination of the hierarchy depends on 1–3 oscillations which have a much shorter wavelength and so may be affected by such a substructure in the reactor spectrum [14], an effect which may even be amplified by the self-calibration of Ref. [1].

The reactor neutrino experiment JUNO will have a very different baseline and total reactor flux from Daya Bay. This leads to different oscillation probabilities. However, the different oscillation probabilities only affect the normalization of the number of events observed in each bin, and not the fractional uncertainty in the reactor flux. Therefore, ignoring the somewhat distinct isotope ratios, the fractional uncertainty in the spectrum at each bin at JUNO will be equal to that at Daya Bay.

To estimate the effect of the unknown spectrum on the determination of θ_{12} , we proceed as follows. First, we determine the shape of the deformation of the reactor spectrum which would simulate in a shift

$$\theta_{12} \to \theta_{12} = \theta_{12} + \delta \theta_{12} \tag{3.1}$$

at JUNO. With a single detector JUNO can never distinguish such a shift in the reactor spectrum from a shift (3.1) in θ_{12} . We fix the value of $\delta\theta_{12}$ such that such a shift in the reactor spectrum fits Daya Bay's determination of the spectrum with $\chi^2 = 1$, using the uncertainties reported in Ref. [25]. This yields an expected systematic shift in JUNO's measurement of $\sin^2(2\theta_{12})$ of

$$\delta(\sin^2(2\theta_{12})) = 0.0035. \tag{3.2}$$

Note that the various degeneracies between the reactor flux uncertainty and uncertainties in the mixing angles, backgrounds, etc. do not affect this calculation, because the χ^2 value of the expected spectrum at JUNO with the shifted reactor flux is equal to 0, since the shift in the spectrum has been chosen such that it can be precisely compensated by a shift in θ_{12} .

3.2. Effect of all other sources of uncertainty

The uncertainty in the reactor flux is not responsible for all of the expected uncertainty in θ_{12} . To determine other contributions to the precision of a measurement of $\sin^2(2\theta_{12})$, we fix the reactor flux to the model of Ref. [12] and use the expected data set to determine the value of $\sin^2(2\theta_{12})$ for which, when choosing the pull parameters of Sec. 2 to minimize χ^2 (defined in Eq. (2.3)), one obtains $\chi^2 = 1$ after 6 years. We recall that the expected dataset, also called the Asimov dataset, does not include statistical fluctuations. We recall that this method reproduces the standard 1σ confidence interval *including* statistical fluctuations for the following reason. When one includes statistical fluctuations, to determine the confidence interval for the determination of θ_{12} one needs to calculate the value of θ_{12} for which the value of a χ^2 fit to the data is greater than that of the χ^2 fit to the best fit θ_{12} by one unit, in other words including statistical fluctuations the 1σ confidence interval is the region in which $\Delta \chi^2 \leq 1$. However, it can be shown that, assuming Gaussian distributions for all variables, this is equivalent to the range of θ_{12} values for which $\chi^2 \leq 1$ for a fit of the given spectra to the best fit spectra *without* statistical fluctuations [26].

We assume that the background can be rejected with an efficiency \mathcal{E} , yielding a fractional dead time τ . The details of the veto strategy have no effect on our analysis, only the rejection efficiency and the dead time. Various fractional dead times are considered. The number of ⁹Li events observed will be of order 10⁵ and so we assume a normalization uncertainty of only 1%, although we have checked that our results change little if this is relaxed. The 51% of ⁹Li decays which produce a neutron are not removed by our double coincidence cut. These decay via

$${}^{9}\text{Li} \rightarrow {}^{9}\text{Be}^{*} + e^{-} + \overline{\nu}_{e} \rightarrow n + 2\alpha + e^{-} + \overline{\nu}_{e}.$$
(3.3)

The e⁻ spectrum can be calculated precisely using Fermi's theory of β decay. As 90% of these decays use a low energy (less than 3 MeV) excited state ⁹Be^{*}, the neutron and α energies are



Fig. 2. The horizontal axis is the ⁹Li rejection efficiency. Each curve represents a different dead time, in ascending order from 0% to 50% in steps of 10%. *Left*: The uncertainty σ in the best fit value of $\sin^2(2\theta_{12})$, assuming a perfectly understood reactor spectrum, optimizing all pull parameters to minimize χ^2 . *Right*: The sum in quadrature σ_{tot} of the uncertainty σ and the shift $\delta(\sin^2(2\theta_{12}))$.

quite low. At low energies, their quenching factors are large. For example the quenching factor of the neutron is about five times that of the electron. As a result the α create negligible scintillation light, while the neutron contributes about 5% of the visible energy. As a result, while the uncertainty on the neutron spectrum is quite large, its contribution to the uncertainty in the shape in the total spectrum is very small. This motivates our crude approximation that the shape of the observed energy spectrum is known precisely. The ⁸He background is similar to the ⁹Li background, but it is smaller and only 16% of decays yield neutrons. As a result, the ⁸He background is suppressed by a factor of 30 with respect to the ⁹Li background [19] and so we ignore it.

The total number of events is obtained by rescaling the measurement of Daya Bay, using global fit mixing angles and mass splittings to remove and put back oscillations, via a procedure described in Ref. [27]. We also assume that the nonlinear energy response of the detector is perfectly understood, although in practice the uncertainty in the nonlinear energy response will yield a significant contribution to the uncertainty in θ_{12} , which according to some studies [10] can, depending on the nonlinear response model, be as large as the contribution from the current uncertainty in the reactor spectrum studied here.

3.3. Final results

This procedure yields the uncertainty in θ_{12} not including the contribution from the uncertain reactor spectrum. The resulting 1σ uncertainties are summarized in the left panel of Fig. 2. In the right panel we add the result in quadrature to $\delta(\sin^2(2\theta_{12}))$ to obtain the final uncertainty $\sigma_{tot}(\sin^2(2\theta_{12}))$. As can be seen, using the recent measurements [23,25] one can reduce the uncertainty in $\sin^2(2\theta_{12})$ to about 0.5%, which is roughly in line with the stated goals of the experimental collaboration. A more precise measurement of the reactor spectrum in the future may reduce this [14], but not beyond the uncertainty displayed in the left panel of Fig. 2.

To determine the precision of a measurement of $\sin^2(2\theta_{12})$ if the third and fourth Taishan reactors are not built is straightforward. These account for 26% of the total thermal power expected at the Taishan and Yangjiang reactor complexes. Therefore one can read the resulting uncertainties off of Fig. 2 by replacing the dead time τ , which corresponds to the color of the curve, by

$$\tau' = 0.76\tau + 0.24. \tag{3.4}$$

4. Remarks

At first glance the fact that our final precision is of the same order as that obtained in previous studies, such as Refs. [9,10], might suggest that this analysis has been trivial. However we would

like to point out that this coincidence is accidental, caused by the fact that the theoretical uncertainties of Ref. [12] are similar in magnitude to last year's observational uncertainty [23,25]. Had we used older data, or last year's data from Double Chooz [24] then the new uncertainty would have been much larger. Indeed the two analyses are quite different. Traditional estimates of the precision of a measurement of θ_{12} , such as that in Ref. [10], are quite precise as they use the uncertainty in [12] for which the full covariance matrix is given. However, for an analysis using the theoretical spectrum of Ref. [12], we claim that they are nonetheless inaccurate as that uncertainty was always intended as a lower bound and was argued in Sec. 2 to be smaller than the true uncertainty by a factor of four. On the other hand, as the uncertainties in our analysis are observational, there is no such bias. Nonetheless, as we do not have a covariance matrix for these uncertainty of JUNO's measurement of θ_{12} is lower than may be expected were JUNO to run today. On the other hand, Daya Bay, RENO and Double Chooz continue to improve the precision of their measurements of the reactor flux, which will reduce the uncertainty in θ_{12} which will be attained by JUNO, but not beyond that reported in the left panel of Fig. 2.

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