NEOS Data and the Origin of the 5 MeV Bump in the Reactor Antineutrino Spectrum

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NEOS data and the origin of the 5 MeV bump

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We perform a combined analysis of recent NEOS and Daya Bay data on the reactor antineutrino spectrum. This analysis includes approximately 1.5 million antineutrino events, which is the largest neutrino event sample analyzed to date. We use a double ratio which cancels flux model dependence and related uncertainties as well as the effects of the detector response model. We find at 3–4 standard deviation significance level, that plutonium-239 and plutonium-241 are disfavored as the single source for the the so-called 5 MeV bump. This analysis method has general applicability and in particular with higher statistics data sets will be able to shed significant light on the issue of the bump. With some caveat this also should allow to improve the sensitivity for sterile neutrino searches in NEOS.

The 5 MeV bump in the reactor antineutrino spectrum was first reported by the RENO collaboration [1, 2] and confirmed by Daya Bay [3] and Double Chooz [4]. Several nuclear physics hypothesis have been put forward to explain the origin of the bump [5–9]. Some argue that the bump could be caused by a particular fissile isotope, *e.g.* uranium-238 [7], whereas other explanations focus on one specific or a small number of fission fragments. Experimentally identifying whether one isotope is predominantly responsible for the bump or not is a crucial step. The NEOS collaboration recently presented first results [10] based on a single-volume, gadolinium-doped, liquid scintillator antineutrino detector of approximately 1 ton fiducial mass at 24 m distance from the core of a power reactor. This measurement constitutes another piece in this puzzle.

The basis for the following analysis is the fact the Daya Bay measurement and the NEOS result were obtained at different effective fission fractions for uranium-235, uranium-238, plutonium-239 and plutonium-241, respectively. The fission fractions in Daya Bay are 0.561, 0.076, 0.307 and 0.056 [11], whereas for NEOS they are 0.655, 0.072, 0.235, 0.038 [12]. The bump in the Daya Bay data is well described in prompt energy by a Gaußian with central value of 4.9 MeV, a width of 0.55 MeV and an amplitude of 10.4%, as can be seen in the left hand panel of Fig. 2. If the bump were equally caused by all four fissile isotopes it should have the same amplitude in both data sets. On the other hand, if the bump is for instance only due to uranium-235, the bump in NEOS should be $0.655/0.561 = 1.17$ times larger, and similarly for all the other fissile isotopes.

The analysis of the bump in either experiment usually relies on a comparison with the Huber+Mueller flux model [13, 14], however this flux model has large uncertainties in itself which limit the obtainable accuracy significantly [15]. Here, we will try to directly compare the Daya Bay spectrum with the NEOS spectrum. Daya Bay has reported a spectrum result which has been "cleaned" of all detector effects by unfolding [11], on the other hand NEOS has presented a result in prompt energy only. The prompt energy in a detector using inverse beta decay is given by $E_{\mathrm{prompt}} = E_{\bar{\nu}} - 0.8\,\mathrm{MeV}$ since an antineutrino of 1.8 MeV, that is at threshold, creates a positron at rest, which will annihilate and deposit twice the electron mass in gamma rays $\sim 1\,\mathrm{MeV}$ in the detector.

For a detector as small as NEOS, energy containment of the positron itself and the 511 keV annihilation gamma-rays is a major issue and thus the relation between prompt and neutrino energy is complex. We try to address this issue by using a double ratio: NEOS not only has published a prompt event spectrum but also the ratio of the measured prompt spectrum to the prompt spectrum predicted by the Huber+Mueller model, R_{NEOS}, shown as black squares in the left hand panel of Fig. 2. For the Daya Bay unfolded spectrum it is trivial to compute the corresponding ratio, $\tilde{R}_{\mathrm{DayaBay}}$ and it is shown as blue circles in the left hand panel of Fig. 2. However this ratio is for a different set of fission fractions. We correct for the difference in fission fractions using the Huber+Mueller model. The resulting correction is small, less than 5% of the total flux and manifests itself as linear slope without any features, as shown as the thick gray line in the left-hand panel of Fig. 2. Assigning a generous bin-to-bin uncertainty of 10% to the Huber+Mueller prediction, the effect on the ratio will be $5\% \times 10\% \leq 0.5\%$, as depicted by a dark gray region in the right-hand panel of Fig. 2. Therefore the large model uncertainties are greatly reduced and can be neglected in the following. We will call the corrected ratio R_{DayaBay}.

We now can form a double ratio $R_{\mathrm{NEOS}}/R_{\mathrm{DayaBay}}$, which in the absence of detector effects would lead to a complete cancellation of the flux model up to the negligible correction for the difference in fission fractions. The NEOS detector response function is unknown to us, but we can make an educated guess towards its general properties and can show that only a small correction results. In Ref. [10] the NEOS collaboration quotes an energy resolution of 5% at 1 MeV and from the information in Ref. [10] we can infer an energy resolution of approximately this form

$$\sigma(E_{\mathrm{prompt}}) = (0.05\sqrt{E_{\mathrm{prompt}}} + 0.12)\,\mathrm{MeV}\,. \qquad (1)$$

There are two types of energy losses through the surface: escaping 511 keV gamma rays and the positron itself can escape as well. Each process has a mean range λ and only events which are closer than λ to the surface can experience a significant energy loss.

The mean range of a 8 MeV positron, λ_{e^+}, in scintillator is approximately 4 cm. For a spherical detector of 1 m^3 volume[1], approximately 15% of the volume lies within λ_{e^+} from the surface. Assuming that one half of all events within this λ_{e^+} thick shell are leaving the detector and that for those events, the energy deposited in the detector forms a flat distribution between 0 and the actual energy of the positron, we obtain a simple, but conservative model of energy losses for positrons.

For the the two 511 keV annihilation gammas the mean range λ_γ, which is due to Compton scattering, is about 8 cm and approximately 28% of the total detector volume is within a shell of this thickness. Using a simple Monte Carlo simulation based on the Compton scattering cross section, we find that indeed about one half of the events generated within a shell of thickness λ_γ will experience energy loss through the surface and we obtain the actual energy loss distribution.

Combining these two ingredients, we obtain our approximate detector response function $D(E_{\text{prompt}}, E_{\text{rec}})$, where E_{rec} is the reconstructed energy, which is shown as a blue line in panel a) of Fig. 1 and for comparison a simple Gaußian response function is shown in green. For $D(E_{\text{prompt}}, E_{\text{rec}})$ (blue curve) the ratio of events which have their energy reconstructed below the true energy to those which have it reconstructed above is 1.32, resulting in a mean reconstructed energy of 4.78 MeV for a true energy of 5 MeV.

We now can study the fidelity of the cancellation of detector effects with a toy example. Assume experiment A is subject to the detector response D and sees a bump of 10% amplitude at 5 MeV. For experiment A we form the ratio R_A of the experimental mock data (with bump) to a theory prediction (without a bump) smeared with the same detector response, D. Experiment A corresponds to NEOS. Next, for experiment B we assume that the data is reported as an unfolded result free from detector effects and that experiment B does see the same bump. We form the corresponding ratio R_B of data and theory. In Fig. 1 we show the resulting double ratio R_A/R_B for two different assumptions about the detector response of experiment A. We see, that we misreconstructed the size of the bump in terms of the double ratio by less than 0.01. We also see that two quite different detector response models, a simple Gaußian versus a model with significant surface energy losses, yield an estimate of the residual effect within a factor of 2 of each other. We will include the 0.01 error in the subsequent analysis despite the fact that this error is about ten times smaller than the errors resulting from statistics in NEOS and Daya Bay, thus even if we were to double this number it would have minor impact on the final result. This demonstrates the robustness of the double ratio against detector effects.

[1] This corresponds to roughly 1 metric ton of liquid scintillator.

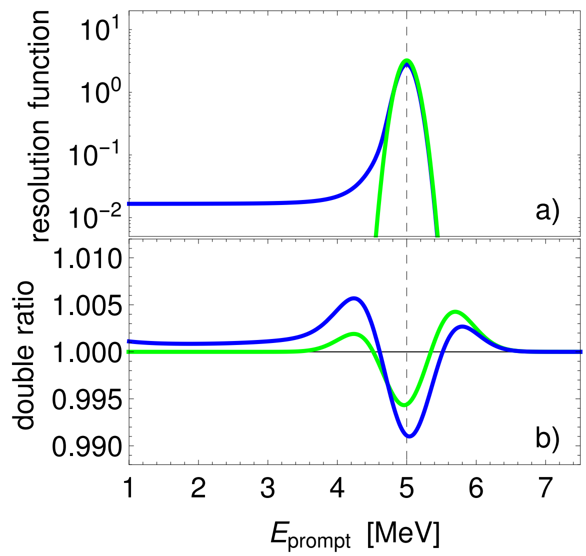

FIG. 1. In panel a) the base-10 logarithm of the resolution function for a true prompt energy of 5 MeV is shown: in green (light gray) a simple Gaußian resolution and in blue (dark gray) a more realistic detector response as explained in the text is used. In panel b) the resulting double ratio is shown for a toy example where there is a bump of same amplitude in the data of both experiment A and the data of experiment B.

Finally, we can look at the resulting double ratio for the actual data $R_{\text{NEOS}}/R_{\text{DayaBay}}$, which is shown in the form of black dots in the right-hand panel of Fig. 2. Note, that the absolute flux is left free, so the fact that the double ratio averages to 1 is of no significance. We clearly observe that the bump is largely canceled between Daya Bay and NEOS pointing towards the fact the amplitude and position of the bump in both data sets is very similar. This double ratio would lend itself extremely well to form the basis of a sterile neutrino search in NEOS, freeing NEOS largely from flux model uncertainties, using Daya Bay as far detector for NEOS. The Daya Bay detectors are at a distance where any sterile neutrino oscillation, with a Δm^2 for which NEOS is sensitive, is averaged out. However, since in a sterile oscillation search many peaks and valleys can appear as localized features in the data, our simplistic treatment of the detector response is suspect: the detector response function nearly cancels for the bump search since the amplitude *and* position of the bump in both data sets is very close, see left hand panel of Fig. 2. As explained, this would be not the case

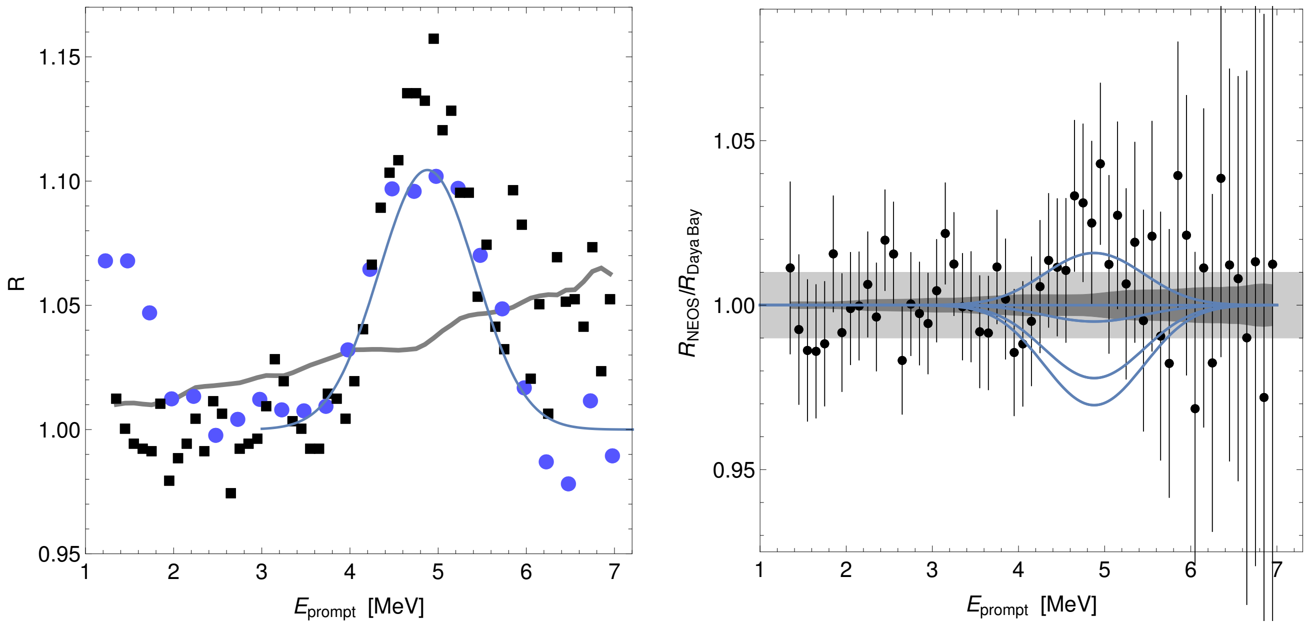

FIG. 2. In the left hand panel, the ratio R of measured spectrum to the Huber+Mueller prediction using the respective fission fractions is shown for Daya Bay as blue circles and for NEOS as black squares. The dark gray line is the correction applied to the NEOS data arising from the different fission fractions in both experiments according to the Huber+Mueller model. The blue curve corresponds to the best fit bump shape in Daya Bay. In the right hand panel, the black dots show the double ratio $R_{\rm NEOS}/R_{\rm DayaBay}$, the error bars are the purely statistical errors from NEOS and the nuisance parameters η, defined in the text, are at their best fit values. The various lines depict the predictions for the bump in the double ratio. The light gray band corresponds to the uncertainty stemming from the NEOS detector response, whereas the dark gray band is the uncertainty of the fission fraction correction and corresponds to 10% of the correction, shown as dark gray line in the left hand panel.

for oscillations, since Daya Bay cannot see any relevant oscillation for the Δm^2 values in question. The double ratio for a sterile analysis, therefore presumably requires a detailed understanding of the detector response and in this case, the cancellation of flux uncertainties will still apply and be very beneficial.

In order to quantify the agreement between the two data sets, we perform a fit to the double ratio of various bump amplitudes. In this fit we include the statistical errors of the NEOS data and the full covariance matrix published together with the Daya Bay unfolded flux [11]. The binning of NEOS data is 100 keV and thus, much finer than the binning of the Daya Bay data of 250 keV. This makes the direct use of the covariance matrix of Daya Bay somewhat difficult in a combined fit. We introduce one nuisance parameter η_i for each of the Daya Bay energy bins by multiplying the bin content with $1+\eta_i$; as these η parameters are varied in the fit we obtain a shifted Daya Bay spectrum. We then use linear interpolation on this shifted Daya Bay spectrum to obtain values for the 100 keV bins of NEOS. The η parameters are constrained in the fit by the covariance matrix $\mathbf{V}^{-1}$ by adding the following term to the χ^2-function $\eta\mathbf{V}\eta^T$. The only physical fit parameter is the bump amplitude in the double ratio where we keep the bump position fixed at 4.9 MeV. Note that black data points shown in Fig. 2 haven been shifted corresponding to the values of η_i found at the best fit point and the error bars shown are the statistical errors of the NEOS data set only.

We use this analysis to test the following five hypotheses: the bump is only in uranium-235 or in uranium-238 or in plutonium-239 or in plutonium-241, and fifth, the bump is equal in all isotopes. The result is shown in Tab. I, the best fit is obtained for $R_{\rm NEOS}/R_{\rm DayaBay}$ at the bump of 1.022 with a χ^2 of 46.7 and the resulting overall goodness of fit is 80%, taking 57-1 degrees of freedom. The standard deviation in Tab. I is obtained by taking the χ^2-value of each model, subtract the best fit and then convert the resulting $\Delta\chi^2$ into standard deviations using a χ^2-distribution with 1 degree of freedom, *i.e.* the number of standard deviations is $\sqrt{\Delta\chi^2}$. The case of the bump being caused by either uranium isotope or equally by all isotopes is clearly preferred over the case where the plutonium isotopes carry sole responsibility. This result is more conclusive than one would expect from the numbers given in [15] because the model uncertainties of the Huber+Mueller model cancel in the double ratio and thus starts to approach the more ideal case of negligible flux errors [16].

The fact that the plutonium isotopes are disfavored as

Isotope	^{235}U	^{238}U	^{239}Pu	^{241}Pu	equal
$R_{\rm NEOS}/R_{\rm DayaBay}$	1.021	0.993	0.971	0.960	1.000
χ^2	46.9	51.6	60.3	66.0	49.9
σ	0.34	1.93	3.27	3.92	1.55

TABLE I. χ^2-values for the the bump being caused by a single isotope or in equal parts by all isotopes. The fit has 57-1 degrees of freedom and the χ^2-minimum is 46.7 and occurs at a value of the double ratio of 1.022.

the sole origin of the bump is at odds with the possibility put forward in Ref. [7], that epithermal fission of plutonium is responsible for the bump. This explanation would have the advantage that it naturally explains why the bump is absent in the integral beta spectra [17–19] since theses measurements were done in a purely thermal neutron flux. Our analysis would still allow uranium-238 to be the sole origin of the bump, but due to the small uranium fission fraction the size of the bump in uranium-238 would have to be of order 2 (!), which should naturally leave an imprint in the integral beta spectrum for uranium-238 fission [20], which is not the case. Thus, the basic riddle of how to accommodate the bump in the antineutrino spectrum without leaving a trace in integral beta spectra remains. It is interesting to note that our analysis slightly prefers uranium-235 as the sole source and that recently it was pointed out that the total inverse beta decay yield of uranium-235 disagrees most with predictions [21]. Also, recent results reported by the RENO collaboration seem to indicate a positive correlation of the bump amplitude with the uranium-235 fission fraction [22], which is consistent with the results presented here. In combination this evidence supports, but does not conclusively establish, uranium-235 as leading contributor to the bump.

Future measurements at research reactors, which exhibit nearly pure uranium-235 fission, clearly will help to distinguish the remaining most likely possibilities: only uranium-235 would predict an amplitude of the bump of about 0.23–0.26, only uranium-238 predicts an amplitude of 0 and equal contribution from all isotopes predicts 0.14 for the amplitude. Note, that these reactors run at fission fractions which are quite different from both NEOS and Daya Bay, thus using the data of NEOS or Daya Bay as a reference will require applying a larger correction for fission fractions based on the Huber+Mueller model and thus a larger fraction of the model uncertainties will apply. Also, these planned experiments will work at a signal of noise ratio very much worse than that of NEOS, which may reduce the statistical power of those experiments. Thus, the impact of these measurements for the question at hand could potentially be significant, but this impact depends on the yet unknown actual performance of the detectors.

In summary, we have shown that a double ratio of experimental data and theory predictions allows to cancel the flux model dependence and related uncertainties and does not rely on accurate modeling of the detector response. Based on a combined analysis of NEOS and Daya Bay data we find with respect to the 5 MeV bump, that the two plutonium isotopes are disfavored as sole source of the bump at approximately 3–4 standard deviations. The Daya Bay data set used here corresponds to about 1,200,000 events and the NEOS data set corresponds to 300,000 events, in combination this is the largest number of neutrino events analyzed jointly to date. It took only 6 months to accumulate the NEOS data and thus it is conceivable that this data set could quadruple in size, and by that, reducing the statistical errors in NEOS by a factor of 2. This could push the ability to distinguish the sole uranium-235 hypothesis from the case of equal contributions from all fissile isotopes above the $3\,\sigma$ level and thus would allow to either establish or to refute uranium-235 as the single most important contributor to the 5 MeV bump.

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