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Status of the Prediction of Reactor Anti-neutrino Spectra

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Abstract. New generation neutrino physics experiments at reactors have recently determined the value of the $\theta_{13}$ mixing angle. Even though their principle is to use multiple detectors allowing to minimize the influence of reactor and nuclear physics ingredients on their results, these ingredients cannot be totally eliminated. They include reactor simulations, but also new computations of reactor anti-neutrino energy spectra. Recently, after a new computation of the reactor anti-neutrino energy spectra, based on the conversion of integral data of the beta spectra from $^{235}\text{U}$, and $^{239,241}\text{Pu}$, a deficit of reactor anti-neutrinos measured by short baseline experiments was pointed out. This is called the reactor anomaly, a new puzzle in the neutrino physics area. Since then, numerous new experimental neutrino projects have emerged. In parallel, computations of the anti-neutrino spectra independent from the ILL data would be desirable. One possibility is the use of the summation method, summing all the contributions of the fission product beta decay branches that can be found in nuclear databases. Studies have shown that in order to obtain reliable summation anti-neutrino energy spectra, new nuclear physics measurements of selected fission product beta decay properties are required. Lately, the first integral measurement of the beta spectrum associated to fast fission of $^{238}\text{U}$ has been performed. Even more recently, the question of the influence of forbidden decays in the determination of reactor anti-neutrino energy spectrum has been raised. At this conference, we will present the methods used to compute reactor anti-neutrino energy spectra, the recent published developments on the topic, remaining open questions and some experimental outlooks.

1. Introduction
Since the last 15 years research in neutrino physics has been very prolific in results, with the determination of most of the oscillation parameters, with the exception of the $\theta_{13}$ mixing angle and the $\delta_{CP}$ phase. Up until 2011 only an upper bound for $\theta_{13}$ was given by the Chooz experiment [1]. Modern accelerator and reactor experiment could tackle the measurement of $\theta_{13}$ in a complementary way. Experiments using reactor anti-neutrinos can perform a clean measurement independently of most of the other parameters, and independently from the $\delta_{CP}$ value, while experiments using accelerator-produced neutrinos and anti-neutrinos can bring information on both parameters. Indeed in 2011, Minos [2] and T2K [3] provided the community with indications of a non-zero $\theta_{13}$ mixing angle through appearance of electron neutrino events in their detectors. The first reactor experiment to release results was Double Chooz, in November 2011 [4]. These results were followed by evidences by Daya Bay [5] and [6] in early 2012. The principle of the new generation reactor anti-neutrino experiments quoted above is to use a detection site near reactor cores to measure the emitted anti-neutrino spectrum at a location where the oscillation has not yet occurred, while a far site will measure the spectrum at the oscillation maximum.
The two sites contain one or several identical detectors so as to cancel most of the detection systematic errors. With the advent of new generation reactor anti-neutrino experiments, re-investigation of reactor anti-neutrino spectra was carried out during the last years. Indeed even with multi-site experiments, one cannot make a measurement fully independent from a spectrum prediction unless having detection sites filling the isoflux condition. With nuclear power plants containing six reactors such as Daya Bay and Reno this condition is not possible to fulfil. In the case of the Double Chooz experiment, the first phase of the experiment takes data with its far detector only and thus its results arise from the comparison of the measurement to a prediction of the anti-neutrino spectrum emitted by the Chooz reactor cores. In its second phase, with the two reactors of the plant in operation, a correction due to non-isoflux conditions will be required as well. The recent re-investigation of the reactor anti-neutrino spectra shed the light on the “reactor anomaly” [7], a deficit in the reactor anti-neutrino flux evidenced in a reanalysis of the short baseline ($\leq 100$ m) experiments at reactors, due to an upward shift of the normalization of the newly converted anti-neutrino spectra [8, 9]. Several explanations could be invoked, and neutrino physicists have started to chase the existence of sterile neutrinos in the $\Delta m^2 \approx 1$ eV$^2$ region with new experimental projects; at research reactors, but also accelerators and with intense radioactive sources [10]. Nuclear physicists have started to investigate possible uncertainties in the calculation of reactor anti-neutrino spectra, and alternative calculations using nuclear data could be desirable, being independent from the unique measurements of integral beta spectra at ILL in the 80s [11] on which the newly converted spectra rely. In this paper, we will review briefly the actual two main methods employed to compute reactor anti-neutrino spectra, and summarize the on-going discussions regarding these calculations.

2. New Converted Spectra
Taking advantage of the numerous information present nowadays in the nuclear databases [8], the first re-computation of the reactor antineutrino energy spectra relied on the use of nuclear data, with the so-called summation technique (Summation Method, called here “SM”), which will be detailed in the next section. The obtained beta energy spectra for the main fissible isotopes were compared with the integral beta spectra precisely measured by Schreckenbach’s team at the ILL research reactor [11]. The comparison showed an agreement at the 10% level, which was not sufficient for neutrino physics experiments. The high energy part of the spectra is over-estimated by the SM and some shape distortions are observed. This trend is compatible with the so-called Pandemonium effect [12]. Interested readers can refer to [8, 13] for further explanations. Benefiting from the gathered nuclear data, the conversion method (“CM”) of the ILL beta integral data was then revisited in order to obtain more precise antineutrino spectra. The conversion procedure consisted originally in fitting the integral beta energy spectra with 30 effective beta branches in order to convert them. The new method used most of the experimental beta branches given by the nuclear databases and fitted 90% of the ILL beta spectra with them, fitting the 10% remaining part with 5 effective branches [8]. Thanks to this new method, the correction to the Fermi theory could be applied at the branch level and the real charge ($Z$) distribution of the fission products could be taken into account, replacing the mean $Z$ fit that was not accurate enough. These corrections led to a 3% normalisation shift upward w.r.t. the antineutrino spectra obtained in [11], triggering the “reactor anomaly” quoted above [7]. Huber revisited the CM in parallel and found similar results [9]. Several possible explanations can be invoked to explain the newly observed deficit of reactor antineutrinos at experiments placed closer than 100m away from reactor cores. There is a large uncertainty associated to the weak magnetism term entering in the computation of beta decay spectra, which could change the normalization of the predictions of the detected antineutrino flux if revealed too far from the adopted value [9]. In addition, these converted spectra rely entirely on the normalization of the ILL data, for which no other measurement exist. These data are still nowadays the data.
of reference for reactor neutrino experiments. The third potential explanation is the presence of short baseline oscillations, with the mixing of the three standard neutrino flavours into one or two sterile neutrinos [7, 10]. In this context, new measurements or alternative methods to compute the antineutrino energy spectra would be desirable.

3. On the Nuclear Data Side: Summation Method

The anti-$\nu$ spectrum associated with one of the 4 fissioning isotopes in a moderated reactor can be computed as the sum of the contributions of all fission products thanks to the use of the full information available per nucleus in Nuclear Databases (NDB). The $\beta/\bar{\nu}$ spectrum per fission of a fissible isotope $S_k(E)$ can be broken-up into the sum of all fission product $\beta/\bar{\nu}$ spectra weighted by their activity $A_{fp}$

$$S_k(E) = \sum_{fp=1}^{N_{fp}} A_{fp} \times S_{fp}^b(Z_{fp}, A_{fp}, E_{0fp}, E)$$ (1)

Eventually, the $\beta/\bar{\nu}$ spectrum of one fission product is the sum over the $b$ branches of all $\beta$ decay spectra (or associated $\bar{\nu}$ spectra), $S_{fp}^b$, (in eq 1), of the parent nucleus to the daughter nucleus weighted by their respective branching ratios. To calculate these quantities, we used the MCNP Utility for Reactor Evolution (MURE) code [14, 21] to extract the fission rates and the fission product activities as a function of time. The Fermi theory has been implemented in MURE in order to calculate the $\beta/\bar{\nu}$ spectrum, $S_{fp}^b$, of each $b$ branch of the $fp^{th}$ fission product. $BR_{fp}^b$, $Z_{fp}$, $A_{fp}$ and $E_{0fp}^b$ have been extracted from the selected NDB.

The $\beta$ spectrum $S_{fp}^b$ in eq. 1 is derived from the Fermi theory taking into account Huber’s prescriptions for the treatment of corrections to be applied to the calculation [9]. In these corrections, two of them should be underlined here for the sake of the understanding of present uncertainties associated to anti-neutrino spectra. We have mentioned in the previous paragraph the weak magnetism correction. This correction arises from the fact that the decaying quark is not free but bound in the nucleon. The weak magnetism correction acts on the spectral shape as a slope as a function of energy, and its average value can be deduced from the magnetic dipole $M1$ gamma decay width in isobaric analogue states, under the CVC hypothesis. Unfortunately, the required nuclear structure knowledge is limited to a few nuclei, the majority of which being lighter than fission fragments. The representativity of this average value can then be questioned, that is the reason why the weak magnetism correction term is a major source of theory uncertainty. Another source of uncertainty affecting potentially the shape of anti-neutrino spectra is the type of the beta transition. Beta decay follow angular momentum selection rules that can be found in numerous textbooks. We just recall here briefly the main definitions for clarity sake. The beta decay transitions are classified in allowed and forbidden transitions for respectively a zero and a non-zero angular momentum taken by the electron-anti-neutrino pair. If the spin of the electron-anti-neutrino pair is one, the transitions are called Gamow-Teller transitions, while if it is zero they are called Fermi transitions. The forbidden transitions have a weaker rate than allowed ones. In forbidden transitions, the degree of forbiddenness is given by the value of the angular momentum, $L=1$ means then a first forbidden transition. First forbidden transitions can be a mix of Fermi and Gamow-Teller transitions, except the one corresponding to a total angular momentum, sum of the angular momentum and of the spin of the pair, equal to two. In this case, these transitions can be only of Gamow-Teller type, they are thus called first forbidden unique transitions. These definitions apply to higher values of the angular momentum of the pair. The shape of forbidden transitions beta energy spectra are affected by energy dependent transition nuclear matrices. The forbidden unique transition beta spectral shapes are well determined, while the non-unique ones require to compute the nuclear
matrix elements with microscopic nuclear structure models on a case by case basis. We will see in the next paragraph, that forbidden non-unique transitions entering in the composition of the reactor anti-neutrino spectrum, could be an additional source of uncertainty [15].

The last ingredient required to compute our calculation with the SM are nuclear data bases which contain all the nuclei information. We have determined a selected choice of NDB. Details can be found in [16, 13]. The choice was carefully made in order to avoid as much as possible Pandemonium-biased data. The Total Absorption Spectroscopy technique is an alternative to the use of Ge detectors allowing to circumvent the Pandemonium effect [17, 18].

The final calculated spectra obtained with the SM for $^{235,238}\text{U}$ and $^{239,241}\text{Pu}$ with 100 keV bins and with the last TAS data can be found in [13]. They are the last up-to-date predictions for these spectra which offer a more precise shape than before [11]. A comparison with the last Huber’s computations over the range 2 to 8 MeV has also been proposed. It shows reasonable agreement in the normalization and shape. We reach at maximum 10% discrepancy up to 7 MeV.

Figure 1. Ratios of the new predicted spectra obtained with and without the last TAS data presented in [17] and extracted from [13].

In Fig. 1, the ratio of the new predicted spectra and the ones obtained with the same data set but the latest TAS data for $^{102,104,105,106,107}\text{Tc}$, $^{101}\text{Nb}$ and $^{105}\text{Mo}$ published in [17], previously simulated with JEFF are presented and illustrate how strongly the Pandemonium effect affects the global anti-$\nu$ energy spectra of $^{235,238}\text{U}$ and $^{239,241}\text{Pu}$. A noticeable deviation from unity (maximum 8% decrease) is obtained for $^{239,241}\text{Pu}$. We observe a maximum of 3.5% deviation for $^{238}\text{U}$. For $^{235}\text{U}$, as these nuclei have a small contribution to its spectrum, the effect is smaller than 1.5% at $\sim 3\text{MeV}$. Moreover, by convolution with the detection cross section (inverse beta decay), the resulting $\bar{\nu}$ flux corresponding to pure fissions of $^{235}\text{U}$, $^{239}\text{Pu}$, $^{241}\text{Pu}$ and $^{238}\text{U}$ is 99.1%, 94.53%, 94.76% and 98.09% respectively relative to previously obtained flux. It stresses again the importance of the Pandemonium effect and the necessity to multiply TAS data measurements to improve the predictiveness of the method. This is emphasized by the fact that the summation method is the only predictive method that can be used to compute anti-neutrino energy spectra associated to any reactor fuel type. These predictions are necessary if one wants to study the potential use of anti-neutrino detectors for reactor core monitoring.
Indeed neutrinos exhibit unique features that have been underlined by the IAEA [?] and that could make of their detection a potential new safeguards tool. Several groups worldwide carry out detector developments to this purpose [20], as well as dedicated reactor simulations [21].

4. Recent Developments

Recently the integral beta energy spectrum arising from $^{238}$U fast fission was determined by Haag et al. [22] relatively to the ILL $^{235}$U energy spectrum from [11]. In this way, the systematic errors of the new measurements are strongly reduced, while the obtained $^{238}$U spectral shape is strongly correlated to the $^{235}$U beta energy spectrum measured with the BILL spectrometer. After a simple conversion procedure, the anti-neutrino spectrum is given in 250 keV bins in the range from 2.875 MeV to 7.625 MeV with an energy-dependent error of 3.5 % at 3 MeV, 7.6 % at 6 MeV and ≥14 % at energies ≥7 MeV (68 % confidence level). Furthermore, an energy-independent uncertainty of 3.3 % due to the absolute normalization is added. Compared to the generally used summation calculations, the obtained spectrum reveals a slight spectral distortion of 10 % but returns the same value for the mean cross section per fission for the inverse beta decay. One should note that this new measurement is a major outcome for the determination of reactor anti-neutrino energy spectra, as up until now, the only determination of the $^{238}$U anti-neutrino energy spectrum was relying on calculations. On the neutrino physics side, the result is not significantly different enough from the calculations previously used to question the present neutrino physics results like the reactor anomaly or the Double Chooz phase one results on $\theta_{13}$. One should notice that as the new $^{238}$U spectral measurement has been performed relatively to the ILL $^{235}$U one, its absolute normalization is fully correlated with the one of the latter spectrum, and thus cannot confirm or infirm the normalization of ILL spectra, which is a strong ingredient of the reactor anomaly, uncorroborated by any measurements as they are unique up until now. In addition, the remarkably good agreement [23] found between the measurement and the summation method spectra from [8, 13] gives confidence to a certain extent on the nuclear physics ingredients entering in summation method spectra.

The agreement is not good enough, though, to eliminate all sources of nuclear physics uncertainties affecting the shape of anti-neutrino spectra. Indeed, in addition to the Pandemonium bias affecting some of the important nuclear data entering in the calculation of anti-neutrino spectra, some other nuclear physics uncertainties could affect both the spectra built with the conversion and the summation methods. Recently, a publication by Hayes et al. [15] pointed out that out of ≃6000 beta decay transitions, about 1500 are forbidden transitions. Phase space factor and Weak Magnetism expressions have to be modified for Forbidden non-unique transitions, and the corrections are not the same for beta and antineutrinos. Even the converted spectra in which the beta spectrum shape is fixed to the ILL data, could be affected if the Forbidden non-unique transitions happened to be contributing importantly to the anti-neutrino spectra depending on which operator among the possible ones dominate the transitions. Without detailed nuclear structure information there is no method of determining which operators determine the 1500 forbidden transitions. If significant contribution for forbidden non-unique transitions is found in the decays of the fission products, Hayes et al. say that the uncertainty associated to the conversion may be greater than 5% over the whole energy range. Ratios of antineutrino spectrum to the original ILL spectrum allowing different operators to dominate the non-unique forbidden transitions were computed showing that the forbidden transitions introduce an operator dependent distortion of spectrum. In reality there will be a mixture of these and other operators.

Recently, a workshop was organized in Seattle in Nov. 2013 [24] in order to gather the nuclear physics community to discuss about the questions raised by these recent nuclear data studies, in the context of the reactor anomaly. In the following, we give a few outcomes of the workshop. As regards converted spectra, the largest uncertainty [9] comes from the weak magnetism term.
as explained in the previous sections. Here we could expect that some constraints will come from
precised reactor antineutrino experiments (DB, DC, Reno) with a precise measurement of the
reactor anti-neutrino energy spectrum shape with their near detectors. This will depend on the
systematic error achievable by these experiments on their detection energy scale, since an error
in the energy scale acts as a slope on the energy spectrum, exactly like the weak magnetism
term. It was noted during the workshop that large log(ft) contribute importantly to the spectra
(30%) but we don’t know yet how many of them are forbidden non-unique transitions, nor the
spin/parity of the transitions. A survey is thus required from nuclear physicists. Potential effects
of compensation that would mitigate the impact of these transitions in the full conversion of
the ILL spectra were also not computed up until now. An agreement on the expressions of the
corrections to Fermi theory should also be found in the following months, as several expressions
have been found in the literature [25]. Agreement on a short list of important contributors [27]
was found to re-measure to correct from the Pandemonium bias in the databases is established,
experiments are on-going in Europe and in the US [26, 27]. The Pandemonium bias distorts
largely the Summation Method spectra which need to be corrected before using them, or should
be used with a estimate of their present error bars. A survey of forbidden non-unique cases
for which the shape of the beta spectra were measured will be performed by nuclear physicists.
The status of fission yields needs to be assessed too [28]. Overall the good agreement with Nils
Haags measurement of $^{238}$U integral beta energy spectrum [22] gives confidence on the present
calculations performed with nuclear data.

5. Conclusions
The improvement of the calculations of reactor antineutrino energy spectra is still a challenge
for both fundamental and applied neutrino physics. The ILL data are up until now the only and
most precise measurements, considered as a reference in neutrino physics. The newly converted
anti-neutrino spectra exhibit a normalization shift w.r.t previous anti-neutrino spectra which led
to the reactor anomaly [7]. Independent evaluations of the reactor spectra could provide new
constraints on the existence of light sterile neutrinos. A possible alternative could be to compute
these spectra with the summation method, based on the nuclear data of the fission products
nuclear properties. It was shown that the Pandemonium nuclei play a major role in the estimate
of the anti-neutrino spectra using the summation method and that TAS measurements of these
nuclei could allow us improving drastically the predictiveness of these spectra. An experimental
program is on-going with this objective. The possible strong influence of first forbidden non-
unique beta transitions on the shape of converted anti-neutrino spectra was also evoked. The
inclusion of the shape distortion due to first forbidden non-unique transitions should be tested
in the ILL data conversion procedure before drawing any definite conclusions. An effort to
provide a summary of the situation regarding these spectra has been launched [24], gathering
the neutrino and nuclear communities. The determination of reactor anti-neutrino spectra has
a wide interest as it is also mandatory for using anti-neutrino detection for reactor monitoring
[19] for safeguards purposes.

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