Atomic effects in reactor antineutrino spectra calculation

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Abstract. To predict and interpret the results of reactor antineutrino experiments, precise theoretical knowledge of the antineutrino spectrum is needed. Reactor antineutrinos are produced in beta-decay of fission products, so, in general, any correction to individual beta-spectra will show up in the resulting antineutrino spectrum. We discuss the influence of atomic effects on reactor antineutrino spectra. We note that these effects may be particularly important for the conversion method, which is based on the transformation of experimental electron spectra.

1. Introduction

Nuclear reactors are the most powerful sources of electron antineutrinos. To predict and interpret the results of reactor antineutrino experiments, precise theoretical knowledge of the antineutrino spectrum is required. Recent interest to accurate calculation of antineutrino spectrum is related, in particular, to the reactor antineutrino anomaly [1] and the 5 MeV ”bump” [2, 3, 4].

Reactor antineutrinos are produced in the following way. In the reactor core, fission of uranium and plutonium isotopes takes place. The fission fragments (usually two) have a large neutron excess and undergo a series of nuclear beta decays

\[(A, Z) \rightarrow (A, Z + 1) + e^- + \bar{\nu}_e,\]  
(1)

where \((A, Z)\) is a nucleus with the atomic mass number \(A\) and number of protons \(Z\), \(e^-\) is the electron, \(\bar{\nu}_e\) is the electron antineutrino. The main contributing fuel isotopes are U-235, U-238, Pu-239 and Pu-241. On average, 5.5 antineutrinos per fission are produced. These antineutrinos have energies of up to about 10 MeV (for more details see, e. g., [5]).

Reactor antineutrinos are usually detected via inverse beta decay (IBD) process

\[\bar{\nu}_e + p \rightarrow e^+ + n\]  
(2)

where \(p\), \(e^+\) and \(n\) are the proton, the positron and the neutron. The antineutrinos with energies lower than the IBD threshold \(E_{thr} = 1.806\) MeV are not detected. Note that in reactor experiments one actually measures the IBD cross section averaged over the antineutrino spectrum \(<\sigma_{IBD}>>;\) it is this quantity that has to be compared with theoretical predictions. However, the cross section of (2) can be calculated with high accuracy (see [6] for more details), so the uncertainties in the theoretical value of \(<\sigma_{IBD}>\) are due to uncertainties in the reactor spectrum.
There are two main ways to calculate the spectrum of reactor antineutrinos: the summation method (also called \textit{ab initio}) and conversion method. Here we discuss some issues related to these methods, in particular related to atomic effects.

2. Beta spectrum calculation

The electron spectrum can be written in the following form:

\[ N(E_e) = K p_e (E_e + m_e) (E_e - E_0)^2 F(Z, E_e) H(E_e) L(Z, E_e) \times \]
\[ \times C(Z, E_e) G\beta(Z, E_e) B(E_e) S(Z, E_e) C_e(Z, E_e) C_{exch}(Z, E_e). \]

Here \( E_e, m_e, p_e \) are the electron kinetic energy, mass and momentum, \( E_0 \) is the endpoint energy, \( K \) is a normalization constant.

The Fermi function \( F(Z, E_e) \) describes the effect of nuclear Coulomb field on the outgoing electrons. In the case of forbidden decays one has to take into account the shape factor \( H(E_e) \), which depends on nuclear matrix elements. The other factors are corrections due to finite electromagnetic size of the daughter nucleus \( L(Z, E_e) \), finite weak size of the mother nucleus \( C(Z, E_e) \), radiative effects \( G\beta(Z, E_e) \), weak magnetism \( B(E_e) \), screening \( S(Z, E_e) \), atomic excitations \( C_e(Z, E_e) \) and atomic exchange \( C_{exch}(Z, E_e) \). The overall effect of these corrections on the spectrum is about several percent (see [7, 8, 9] for more details).

To compute the antineutrino spectrum, one has to replace \( E_e \) with \( E_0 - E_e \) in (3) and change the radiative correction for an appropriate one.

Let us briefly describe the atomic effects: screening, atomic excitations and exchange and bound-state beta decay [10]. For all these effect, it is important that beta decay occurs in an atom, not in an isolated nucleus. Screening of the daughter nucleus Coulomb field by the atomic electrons leads reduces the effect of that field on the outgoing electron; it is significant for low-energy electrons and negligible for high energies.

Atomic excitations are transitions of atomic electrons to excited states or into continuum due to imperfect overlap between orbitals of the initial and final atom. The transition to the continuum,

\[ (A, Z) + e^- (\text{bound}) \rightarrow (A, Z + 1) + 2e^- + \bar{\nu}_e, \]

is of particular interest, since one gets two outgoing electrons per decay (and per antineutrino) instead of one. For calculation of antineutrino spectra from individual transitions, the effect is not substantial, because it is relevant to low energies below the IBD threshold.

Atomic exchange takes into account that \( \beta^- \)-electron can be created in a bound state, with a simultaneous transition of an atomic electron into continuum. The effect is significant for neutrinos with energies near the endpoint.

It is also possible that the electron is produced in a bound state, with no outgoing electrons at all

\[ (A, Z) \rightarrow (A, Z + 1) + e^- (\text{bound}) + \bar{\nu}_e. \]

The effect is small for neutral atoms (about 0.1\%) and usually neglected (see [10]). However, it is considerable for ions. The fission fragments are usually produced as ions, since the atomic orbitals change dramatically. Therefore, the process (5) may be significant for reactor experiments.

3. Summation method

This method of obtaining the reactor antineutrino spectrum is based on calculation of individual spectra from all fission products (about 10000 nuclear transitions overall) and their summation, taking into account their activity (see, e. g., [5]). The main drawback of this approach is the lack of information (decay schemes, branching ratios, spins/parities of nuclear states) in the nuclear
databases. Some data on fission yields and nuclear parameters may vary in different databases. Also, the calculations are usually made with the same “usual” assumptions, which is not always justified (see analysis in [11]). Due to all these problems, the summation method usually underestimates the reactor spectrum. The corrections to individual spectra have to be accounted for, but their influence is not as dramatic as the effect of nuclear database uncertainties.

4. Conversion method

The method is based on the relation between electron and antineutrino spectra. First, the electron spectra from fission products of U-235, U-238, Pu-239, Pu-241 are measured. Then they are fitted with about 30 synthetic transitions. Finally, one uses the endpoints and relative weight from the fit to calculate the antineutrino spectra and sums these spectra. One of the problems of this approach is that the measurement of electron spectrum is quite difficult; the errors may significantly alter the result. There are also some computational issues, such as the relation between the bin width and the fitting intervals (see [12] for details). Also, the fitted spectra are usually considered allowed and the corrections to the spectra (some or all) are ignored.

For the conversion method, the differences in normalization of electron and antineutrino spectra may come into play. For instance, the radiative corrections are different; the relevant conversion factor was given in [13]. Another point is related to processes (4) and (5). Due to them effects, one may get two or zero electrons (instead of one) per decay (and per antineutrino). Therefore, the overall normalization of electron and antineutrino spectra will differ.

5. Conclusion

Calculation of reactor antineutrino spectra is essential for neutrino physics. It is desirable to develop the summation and conversion methods, as well as to improve the computational methods for individual beta spectra. In particular, one has to account for the atomic effect more consistently.

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