Atomic effects in reactor antineutrino spectra calculation

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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 needed. Recent interest to accurate calculation of antineutrino spectrum is related, in particular, to the reactor antineutrino anomaly [1] and the 5 MeV "bump" [2]. There are two main ways to calculate the spectrum of reactor antineutrinos: the summation method (also called \textit{ab initio}) and conversion method. Both methods rely on calculation of individual beta-decay spectra. Here we discuss the corrections to beta spectra due to atomic effects and their implications to the reactor spectra.

Beta spectrum calculation
Let us write the electron spectrum in the following form:

\[
N(E_e) = K p_e (E_e - E_0)^2 F(Z, E_e) H(E_e) \times C(Z, E_e) \tau_{\text{excitation}}(Z, E_e) C_{\text{exchange}}(Z, E_e)
\]

(1)

Here \(E_e\) and \(E_0\) are the total electron energy and the endpoint energy, \(p_e\) is the electron momentum, \(K\) is a normalization constant. The antineutrino spectrum is obtained by replacing \(E_e\) with \(E_0 - E_e\).

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 \(H(E_e)\) depending on nuclear matrix elements. The factor \(C(Z, E_e)\) includes electromagnetic and weak finite-size corrections, screening correction, radiative corrections, weak magnetism correction (see [3] for more detail). Imperfect overlap between atomic orbitals of the initial and final atom may cause transitions to excited states or into continuum. This effect, described by correction \(\tau_{\text{excitation}}(Z, E_e)\), is relevant to electrons in a narrow energy range near the endpoint and, thus, is not substantial for neutrino experiments, since the neutrinos are detected via inverse beta decay

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

(2)

with a threshold \(E_{\text{thr}} = 1806\) keV.

Figure 1: Relative effects of atomic excitations, atomic exchange and other corrections on antineutrino spectrum for \(^{144}\text{Pr}\) branch with endpoint energy 2998 keV.

The atomic exchange correction \(C_{\text{exchange}}(Z, E_e)\) takes into account that the electron in \(\beta^-\)-decay can be created not only in a continuous state, but also in a bound state on atomic orbital with a simultaneous transition of an atomic electron into continuum. The effect is significant for low-energy electrons \((E_e < 100\) keV\) and, hence, for neutrinos with energies near the endpoint. Note that it is also possible that the electron is produced in a bound state [4]; the effect, however, is small for neutral atoms (about 0.1\%) and usually neglected. As an illustration, the relative corrections to antineutrino spectrum for \(^{144}\text{Pr}\) branch with endpoint energy 2998 keV are shown on figure 1.

Summation method
This method 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/purities 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 [6]). 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.

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 [7] for details). We are now working on some of these issues. 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 corrections to electron and antineutrino spectra may come into play. For instance, the radiative corrections are different; the relevant conversion factor was given in [8]. Another point is related to the atomic effects, particularly atomic excitations and bound state beta decay. Due to these effects, one may get 2 or 0 electrons (instead of 1) per decay (and per 1 antineutrino). Therefore, the overall normalization of electron and antineutrino spectra will differ.

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.

References