Electron capture and the neutrino mass.

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Abstract. The electron neutrino mass can be determined by electron capture. One expects the largest influence of the neutrino mass on this decay for a small Q value of Q = 2.8 keV for

\[ ^{163}\text{Ho} + e \rightarrow ^{163}\text{Dy} + \nu. \]

The energy of the Q value is distributed to the emitted neutrino and the excitation of the Dy atom. Thus the energy difference between the Q value and the upper end of the deexcitation spectrum is the electron neutrino mass. The electron wave functions are calculated selfconsistently by the Dirac-Hartree-Fock approach for the bound and the continuum states. To extract the neutrino mass from the spectrum is only possible, if the background is reduced relative to the present situation. The analysis presented here shows, that the determination of the electron neutrino mass by electron capture is difficult, but seems not to be impossible.

1. Introduction

The neutrino is one of the least known particles, although it plays a central role in weak interactions. We do not know the mass of the three neutrinos: electron, muon and tauon neutrinos (and antineutrinos) [1, 2, 3, 4, 5, 6, 7, 9]. We do not know their hierarchy. The nature of the neutrinos, Dirac (neutrino different from the antineutrino) or Majorana (neutrino identical with the corresponding antineutrino) is still unknown [10, 11, 12, 13, 14].

The topic of this contribution is the theoretical side of the determination of the electron neutrino mass by electron capture in \(^{163}\text{Ho}\) as developed by the Tuebingen group and coworkers [5, 15, 16, 17, 18]. For the capture

\[ ^{163}\text{Ho} + e \rightarrow ^{163}\text{Dy} + \nu \]

the Q value obtained by a Penning trap measurement by Eliseev et al. [19] (see also [20, 21, 22]) is:

\[ Q = 2.833(30_{\text{stat}})(15_{\text{sys}}) \text{ keV} \]

This means, that electron capture in \(^{163}\text{Ho}\) is only possible from electron orbits bound less than Q = 2.8 keV. So capture is only possible from 3s\(_{1/2}\), M1 with a binding energy 2.128 keV and less bound electron states. In addition the electron orbits in Ho, from which an electron can be captured must have an overlap with the nucleus to react with a proton. The energy of the Q value after capture is distributed over the excitation energy of the Dy atom (one-, two-, three-hole and higher excitations) and the emitted neutrino. The sum of the deexcitation energy can be measured by a bolometer. The maximum bolometer energy yields then the minimum neutrino
energy, which is the electron neutrino rest mass. Thus the neutrino mass can be determined by the difference of the Q-value and the upper end of the bolometer spectrum. The excitation energy of the Dy* is calculated in the sudden approximation. The excitation of the Dy* is then given by the overlap with Ho* with an electron hole in the capture orbit with the different excited configurations $|D>$ in the daughter Dy*.

According to a publication by Intemann and Polock [8] DeRujula and Lusignoli [9] use non-relativistic pure Coulomb wave functions for the electrons in Ho, which do not allow capture from np$_{1/2}$. The effect of the partial screening of the nuclear Coulomb potential by the electron cloud is considered by effective charges. Since in reference [9] the perturbation approach is used to calculate the Dy* wave functions, this requires orthonormal basis functions. Thus ref. [9] uses for each capture process, e.g. from 3s$_{1/2}$ to calculate the Dy* wave functions, this requires orthonormal basis functions. Thus ref. [9] uses for each capture process, e.g. from 3s$_{1/2}$, the same screening factor for all single electron orbits needed in the perturbation approach for this special capture process. Starting from these ”bad” wave functions for Ho ref. [9] calculates as proposed by [8] the bound and continuum electron wave functions for Dy* with the perturbation:

$$H'(r) = +1/r - \int d^3r_1 |\varphi_{3s/4s}(\vec{r}_1)|^2/|\vec{r} - \vec{r}_1|.$$  

(3)

The first term takes into account, that in Dy one has one proton less compared to Ho. The second term originates from the electron hole in the 3s$_{1/2}$ or the 4s$_{1/2}$ state, which are the only hole states considered in ref. [9]. We use here selfconsistent Dirac-Hartree-Fock wave functions calculated specifically for Ho* and Dy* [23, 24, 25]. The continuum electron wave functions in Yb* are determined [26] in the selfconsistent Z-1 = 65 electron potential orthogonal to all 65 bound electrons in Yb.

2. Description of Electron Capture

The spectrum of the decay of the excited $^{163}$Dy* after electron capture in $^{163}$Ho refs. [4, 9] and [5] assuming Lorentzian shapes for the decay resonances are:

$$\frac{d\Gamma}{dE_c} \propto \sum_{i=1,..,N_{\nu}} (Q - E_c) \cdot U_{e,i}^2 \cdot \sqrt{(Q - E_c)^2 - m_{\nu,i}^2} \cdot \left( \sum_{f=f'} \lambda_0 B_f \frac{\Gamma_{f'}}{2\pi} \frac{1}{(E_c - E_{f'})^2 + \Gamma_{f'}^2/4} + \right)$$  

(4)

$$\sum_{f=f';g'<F;g'_{<F}>F} \lambda_0 B_{f'g'<F;g'_{<F}>F} \frac{\Gamma_{f'g'}}{2\pi} \frac{1}{(E_c - E_{f'g'})^2 + \Gamma_{f'g'}^2/4} + \int dk' \lambda_0 B_{f'g'<F;g'_{<F}>F} \frac{\Gamma_{f'g'}}{2\pi} \frac{1}{(E_c - E_{f'g'})^2 + \Gamma_{f'g'}^2/4}.$$

The factor in front of the bracket is the same as for the single beta decay. It reflects the phase space of the emitted neutrino (1). The three expressions in the bracket of eq. (4) describe the decay of the 1-hole $f'$ excitations in Dy*, of the 2-hole excitations $f'$, p' with shake-up of p' to q' into a bound orbit and of 2-holes $f'$, p' states with one electron p' moved to q' into the continuum (shake-off). The last term has as the others a dimensionless strength $dk' \cdot B_{f'g'<F;g'_{<F}>F}$. The transformation to an integral over the energy yields the factor in front of the third term, which can be deduced from eq. (11). Different neutrino mass eigenstates $|i>$ are mixed into the electron neutrino flavor states by $U_{e,i}^2$. The Q-value is given by eq. (2)
from the ECHO collaboration [20, 21, 27, 28, 29]. The excitation energy of the final Dy* is \( E_c \).

The energy \( Q - E_c \) is carried away by the neutrino. \( B_f, B_{f,p'<F,q'q'>F} \) and \( B_{f,p'<F,q'q'>0} \) are the overlap and exchange corrections for the 1-hole, the bound 2-hole and the shake-off 2-hole states. \( \lambda_0 \) contains the nuclear matrix element squared [30]. Eq. (4) yields the spectrum in arbitrary units and must be normalized at one energy to the data. We use the N1, 4s1/2 peak for the normalisation. \( E_f, E_{f,p'} \) and \( E_{f,p';q',q'} > 0 \) are the 1-hole, the 2-hole shake-up and the 2-hole shake-off excitation energies in Dysprosium (see refs. [7] and [10]). \( \Gamma_f, \Gamma_{f,p'} \) and \( \Gamma_{f,p';q',q'} > 0 \) are the widths of the one- and two-hole states and the two-hole states with shake-off in Dysprosium [15, 16, 17, 18].

The overlap and exchange corrections \( B_f, B_{f,p'<F,q'q'>F} \) and \( B_{f,p'<F,q'q'>0} \) are calculated in second quantisation with Dirac-Hartree-Fock (DHF) electron wave functions. This yields automatically the antisymmetrisation and the exchange terms. The antisymmetrized two-hole state in Dy with shake-off is for example:

\[
\left| A_{f',p';q',q'} > 0 \right> = a_f^\dagger a_{p'}^\dagger \cdots a_{f'-1}^\dagger a_{f'+1}^\dagger \cdots a_{p'-1}^\dagger a_{p'+1}^\dagger \cdots a_q^\dagger a_{q'}^\dagger \cdots 0 > \right.
\]

The probability to form a two-hole shake-off state is proportional to \( |G> \) is the DHF groundstate of Holmium):

\[
P_{f',p';q',q'} > 0 = \left| < A_{f',p';q',q'} | a_i |G> \right|^2
\]

3. The electron wave functions in the Dy Continuum.

The selfconsistent Coulomb field for the shake-off electron is in atomic units:

\[
V_{\text{shake-off}}(r) = -\frac{66}{r} + \sum_k \text{occupied } e \ g_k \int d^3r \cdot \frac{|\varphi_k(r)|^2}{|\vec{r} - \vec{r}'|}
\]

\( g_k \)s are the number of bound electrons in the selfconsistent occupied orbits \( |k> = |n, \ell, j> \) of Dy. To determine the potential for the shake-off electrons in Dy one needs the occupied selfconsistent Dirac-Hartree-Fock upper \( P_k(r) \) and lower \( Q_k(r) \) components of the selfconsistent electron wave functions.

\[
\varphi_k(r) \cdot r = (P_k(r);Q_k(r))
\]

\[
V_{\text{shake-off}} \approx -\frac{66}{r} + \frac{65}{r} \cdot [1 - \exp(-a \cdot r)] \ [1/(\text{length} = \text{a.u.})]; \ a = 3.4
\]

We adjust an analytic expression (9) to the DHF potential (see figure 1). The selfconsistent Dy potential for the 66th. electron in the continuum is shown in figure 1 for Dy. For the normalization of the continuum Dirac wave function we follow here this recommendation of Perger and Karrighattam on their page 394 [32]. In the asymptotic expression (10) \( \eta \) is the Sommerfeld parameter, \( \Delta \) the Coulomb phase shift and \( \delta \) takes into account deviations from a pure Coulomb potential. The electron energy in the continuum can be due to energy conservation not larger than the Q-value of 2.8 keV minus the excitation energy of the two hole state.

\[
\int_{r=0}^\infty dr \cdot 2 \cdot \sin (kr - \ell \cdot \frac{\pi}{2} - \eta \ln 2kr + \Delta + \delta) \cdot \\
2 \cdot \sin (k' r - \ell \cdot \frac{\pi}{2} - \eta \ln 2kr + \Delta + \delta) \approx 2\pi \cdot \delta(k - k').
\]
The wave number is connected with the relativistic and non-relativistic energies by the equations:

\[
E_{rel}^2 = c^2 \bar{\hbar}^2 k^2 + m^2 c^4 \rightarrow c^2 k^2 + c^4 \quad (\text{in atomic units}); \quad E_{n-rel} = \frac{1}{2} k^2;
\]

\[
k = \alpha \sqrt{E_{n-rel} (E_{n-rel} + 2 \cdot c^2)}; \quad \text{with } c = 1/\alpha = 137.035999 \text{ in [atomic units].} \quad (11)
\]

4. Shake-off Process.
The overlap between the bound Ho states \(ns_{1/2}\) and \(np_{1/2}\) with \(n \geq 3\) and the continuum wave functions in Dy squared gives the probability for shake-off. We restrict this work to s-wave shake-off, which is expected to be the largest contribution. The s-wave shake-off is given by the overlap \(<n \geq 3, s_{1/2}, Ho | E, s, Dy >\) squared. In the spectrum with 1-hole, 2-hole and shake-off in figure 2 the shake-off contribution is hardly visible. Here and also in ref. [9] only the decay width of the 2-hole states are included. Three hole states can be neglected [17]. The electron in the continuum has an escape width, which is not included.

Figure 2 shows the logarithmic spectrum of the 1-hole, the 2-hole and the s-wave shake-off contributions. The shake-off spectrum can hardly be seen on this scale in the total spectrum.
Figure 2. Theoretical results in arbitrary units of the sum of the one- and two-hole deexcitations compared to the sum of the one-, two-hole and the shake-off deexcitation as measured by the bolometer spectrum (4). The arbitrary units are adjusted to the experimental $N_{1, 4s_{1/2}}$ 1-hole peak. The nature of the one hole states are indicated. The two-hole peaks are by about two orders of magnitudes smaller than the one hole peaks. Shake-off can almost not been seen.

5. Summary

In this contribution I summarized our theoretical work on the determination of the electron neutrino mass by electron capture [5, 7, 15, 16, 17, 18] in $^{163}$Ho to $^{163}$Dy. The energy of the Q-value $= 2.833 \pm 0.05$ keV is distributed to the excitation of Dy and the emission of a neutrino. The recoil of $^{163}$Ho can be neglected. The total deexcitation energy as X-rays and Auger electrons of Dy can be measured in a bolometer. The upper end of the spectrum requires the minimum energy of the neutrino. Thus the difference of Q minus this upper limit of the deexcitation spectrum is the rest mass of the electron neutrino.

We describe the bound states in Ho and Dy by the Dirac-Hartree-Fock approach [23, 24, 25] even including occupations in Dy due to different hole states. The s-wave continuum wave functions in Dy are determined with the Dirac equation in the selfconsistent potential [26]. (See figure: 1 ). The energy of the capture orbit in Ho and the excitations of Dy* including also the continuum states are limited by energy conservation to the Q-value minus the excited one-hole states in Ho* and Q minus the excitation energies in Dy*.

Remaining discrepancies between theory and experiment could be due to configuration mixing not included here. Finally we want to stress, that the accuracy needed to extract the neutrino mass can not be obtained by theoretical calculation alone. One must fit simultaneously the neutrino mass, the Q-value, the excitation energy of the highest resonance, their width and their strength at the upper end of the spectrum to extremely accurate data. For this the present
background of the experimental spectrum has to be drastically reduced. The measurement must probably be done in an underground lab to protect against cosmic rays. This reduces the background as a first measurement in the Modane underground lab in the Fréjus tunnel has shown [33]. If the background can be reduced by one to two orders, it should be enough to adjust only the two parameters, the Q-value and the neutrinos mass, to the upper end of the spectrum for the determination of the electron neutrino mass.

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