Determination of the neutrino mass in $^{163}$Ho.

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Abstract. KATRIN plans to determine the electron anti-neutrino mass in the Tritium decay. Electron capture in $^{163}$Ho can measure the electron neutrino mass supported by the small decay energy $Q = 2.8$ keV $^{163}$Holmium + electron $\rightarrow$ $^{163}$Dysprosium + $\nu$. The decay energy of 2.8 keV is used to emit a neutrino and to excite the Dy atom. The neutrino mass is then given by the difference between the $Q$ value and the upper end of the Dy deexcitation spectrum. The Dirac-Hartree-Fock approach is used for the bound and the continuum states in Holmium and in Dysprosium. The present background must be reduced by at least two orders to extract the neutrino mass from the spectrum. The present work discusses the one- and the two-hole excitations in Dy. The two-hole states are excited by shake-up of an electron into a free bound state and the shake-off into the continuum. The shake-off contribution can practically be neglected. It seems not to influence the neutrino mass determination.

1. Introduction

Although the neutrino is an essential particle for the weak interaction many of its properties are unknown. Unknown are the mass of the three neutrinos and three anti-neutrinos, the hierarchy and the nature of the neutrinos, Dirac (neutrino different from the antineutrino) or Majorana (neutrino identical with the corresponding antineutrino).

The topic of this contribution is the theoretical side of the determination of the electron neutrino mass [1, 2, 3, 4, 5, 6, 7, 9] by electron capture in $^{163}$Ho by the Tuebingen group and coworkers [5, 15, 16, 18]. For the capture

$^{163}$Holmium + bound Electron $\rightarrow$ excited $^{163}$Dysprosium* + Neutrino

the decay energy $Q$ was obtained by a Penning trap measurement by Eliseev et al. [19] in the MPI in Heidelberg ( [20, 21, 22]).

$\text{Decay energy } Q = 2.833(30_{\text{stat}})(15_{\text{sys}}) \text{ keV}$

Electron capture in $^{163}$Ho is only possible from electron orbits bound less than $Q = 2.8$ keV, thus from $3s_{1/2}$, $M1$ with a binding energy 2.128 keV and from $p_{1/2}$, $M2$ with binding energy of 1.8 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. This is only the case for $(n > 2)s_{1/2}$ and the lower relativistic amplitude of the $(n > 2)p_{1/2}$ states. The decay energy of 2.8 keV is shared by the excitation energy of the Dy atom (one-, two-, three-hole and higher excitations) and by the emitted neutrino. The excited Dy decays by X-rays and...
Auger electron emissions. 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 decay energy and the upper end of the Dy deexcitation spectrum. The excitation of the Dysprosium\(^*\), calculated in the sudden approximation, is then given by the overlap with Holmium\(^*\) with an electron hole in the capture orbit with the different excited configurations \(|D>\) in the daughter Dysprosium\(^*\).

A publication [9], which studies also shake-up and shake-off in Holmium capture, uses 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 there 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 \(3s_{1/2}\), the same screening factor for all single electron orbits needed in the perturbation approach for this special capture process independent of the binding energy of the single electron orbits. Starting from these "bad" wave functions for Ho ref. [9] calculates the bound and continuum electron wave functions for Dy\(^*\) with the perturbation:

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

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 Dy\(^*\) are determined [26] in the selfconsistent Z-1 = 65 electron potential orthogonal to all 65 bound electrons in Dy.

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

\[
\frac{d\Gamma}{dE_c} \propto \sum_{i=1,...,N_r} (Q - E_c) \cdot U^2_{e,i} \cdot \sqrt{(Q - E_c)^2 - m^2_{\nu,i}} \cdot \left( \sum_{f=f'} \lambda_0 B_f \frac{\Gamma_{f'}}{2\pi (E_c - E_{f'})^2 + \Gamma_{f'}^2/4} + \right)
\]

\[
\sum_{f=f';p'<F;q'_b>F} \lambda_0 B_{f,p'<F;q'_b>F} \frac{\Gamma_{f',p'}'}{2\pi (E_c - E_{f',p'})^2 + \Gamma_{f',p'}'^2/4} + \int dk' \lambda_0 B_{f,p'<F;q'_b,F} \frac{\Gamma_{f',p',q'}}{2\pi (E_c - E_{f',p',q'})^2 + \Gamma_{f',p',q'}'^2/4}
\]

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 of the bound occupied electron orbits \(f', p'\) with shake-up of \(p'\) to \(q'\) into an empty bound orbit \(q'\) above the Fermi surface \(F\).
The selfconsistent Coulomb field for the shake-off electron is in atomic units:

\[ V_{\text{Coulomb-shake-off}}(r) = -\frac{66}{r} + \sum_{k \text{ occupied}} g'_k \int d^3 r' \cdot \frac{|\varphi_{k'}(r')|^2}{|r-r'|} \]

\( g'_k \)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 relativistic upper and lower Dirac-Hartree-Fock orbitals in Dysprosium with the single electron quantum numbers \( k' \): \( P_{k'}(r) \) and \( Q_{k'}(r) \).

\[ \varphi_{k'}(r) \times r = (P_{k'}(r); Q_{k'}(r)) \]

The normalization of the continuum Dirac wave function is treated in M. E. Rose "Relativistic electron theory" [30] or Walter Greiner "Relativistic Quantum Mechanics" [31]. We follow here this recommendation of Perger and Karrighattam on their page 394 [34]. 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.
Figure 1. 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) in arbitrary units. The units are adjusted to the experimental N1, 4s\textsubscript{1/2} 1-hole peak. For the one hole states the quantum numbers 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.

\[ \int_{r=0}^{\infty} dr \cdot 2 \cdot \sin(kr - \ell \cdot \frac{\pi}{2} - \eta \ln 2kr + \Delta + \delta) \cdot 
2 \cdot \sin(k'r - \ell \cdot \frac{\pi}{2} - \eta \ln 2kr + \Delta + \delta) \approx 2\pi \cdot \delta(k - k'). \]

The wave number is connected with the relativistic and non-relativistic energies by the equations:

\[ E_{n-\text{rel}}^2 = c^2h^2k^2 + m^2c^4 \rightarrow c^2k^2 + c^4 \quad \text{(in atomic units)}; \quad E_{n-\text{rel}} = \frac{1}{2}k^2; \]
\[ k = \alpha \sqrt{E_{n-\text{rel}}(E_{n-\text{rel}} + 2 \cdot c^2)}; \quad \text{with} \quad c = 1/\alpha = 137.035999 \text{ in [atomic units].} \]

4. Electron Shake-off into the Dy Continuum.
The overlap between the bound Ho states ns\textsubscript{1/2} and np\textsubscript{1/2} with n ≥ 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 $<n \geq 3, s_{1/2} | H^0 | E, s, Dy >$ squared. In the spectrum with 1-hole, 2-hole and shake-off in figure 1 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. The electron in the continuum has an escape width, which is not included.

Figure 1 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.

5. Summary
This publication treats the theoretical side of our determination of the electron neutrino mass by electron capture [5, 7, 15, 16, 18] in $^{163}_{67}$Ho to $^{163}_{66}$Dy. The energy of the $Q-value = 2.80 \pm 0.08 \text{ keV}$ is distributed to the excitation of Dy and the emission of a neutrino. The recoil of $^{163}_{67}$Ho can be neglected. The deexcitation 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 [25, 23, 24] 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]. 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.

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