CALORIMETRIC MEASUREMENTS OF $^{163}$holmium DECAY AS TOOLS TO DETERMINE THE ELECTRON NEUTRINO MASS

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ABSTRACT

We compute the spectrum of "calorimetric" energy in the electron capture decay of $^{163}$Ho. A calorimetric experiment would yield an excellent determination of the ($^{163}$Ho,$^{163}$Dy) mass difference. The proximity of the spectral endpoint to an atomic resonance makes the fraction of events that are sensitive to a non-zero neutrino mass superior in $^{163}$Ho decay than in Tritium decay.

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The most restrictive limits on electron antineutrino masses

\[ m(\overline{\nu}_e) < 60 \text{ eV (90\% conf.)} \quad [\text{Bergkvist}^1] \] (1a)

\[ 14 \text{ eV} < m(\overline{\nu}_e) < 46 \text{ eV (99\% conf.)} \quad [\text{Lubimov et al.}^2] \] (1b)

result from the analysis of the shape of the electron energy spectrum\(^3\) in \(^3\)H \(\beta\) decay near its maximum energy endpoint. These magnetic spectrometer experiments\(^1,^2\) have an energy resolution comparable to, or larger than, the energy differences between the various atomic (or molecular) states in which the daughter \(^3\)He\(^+\) ion (or ionized molecule) can be left in \(^3\)H decay. Theoretical calculations of the branching ratios into these different final states are needed, since they affect the theoretical shape of the spectrum and thus the experimental \(m(\overline{\nu}_e)\) results. This "molecular interplay" problem\(^4\) can be dealt with either by trusting the theory, or improving the resolution and counting rate to such a level that the contributions of the different decay branches are observable, or performing an entirely different experiment where the problem is absent. J.J. Simpson has chosen the third route and obtains

\[ m(\overline{\nu}_e) < 65 \text{ eV (95\% conf.)} \quad [\text{Simpson}^5] \] (2)

The idea is to implant the \(^3\)H source in a Si(Li) crystal that measures all of the energy released in each decay, but that of the escaping neutrino. The "calorimetric" energy \(E_c\) and the neutrino energy \(E_\nu\) add up to the \(Q\) value (mass difference between the ground state \(^3\)H and \(^3\)He atoms, modified by the small difference of their binding energies to the crystal). The value of \(E_c\) is the sum of the \(\beta\) ray energy and the de-excitation energy of the level in which the daughter atom (or daughter detector!) is left in the decay. The decay branch and de-excitation pattern chosen by a particular event do not affect the value of \(E_c\): there are no atomic or molecular interplay problems.

In a decay process involving neutrinos, the smaller the energy release, the bigger the fraction of the spectrum that is sensitive to a fixed non-zero neutrino mass. In a calorimetric experiment, moreover, the smaller the \(Q\) value the better the energy containment, the smaller the radiation damage. Two nuclides are known to decay with a smaller energy release than \(^3\)H. One of them, \(^{163}\)Ho, decays by atomic electron capture into \(^{163}\)Dy + \(\nu_e\). Two experiments have recently measured the lifetime and \(Q\) value of this decay, with the results\(^*\):

\[^*\] In quoting the results [Eqs. (3)] we have assumed that \((Q - E[M_i])^2 \ll m(\nu_e)^2\)

where \(E[M_i] = 2.05 \text{ keV}\) is the \(M_i\)-electron binding energy in Dysprosium.
\[ Q = 2.58 \pm 0.10 \text{ keV} ; \quad T_{1/2}^1 = (7 \pm 2) \times 10^3 \text{years} \quad \text{[Andersen et al.]} \]  
(3a)

\[ Q = 2.30 \pm 0.15 \text{ keV} ; \quad T_{1/2}^1 = 300^{+500}_{-200} \text{ years} \quad \text{[Yasumi et al.]} \]  
(3b)

to be compared with \( Q(\beta \gamma + ^3\text{He}) = 18.6 \text{ keV}, T_{1/2}(^3\text{He}) = 12 \text{ years}. \)

We envisage the possibility that a calorimetric experiment can be performed with \(^{163}\text{Ho}\) as the source of activity, in an attempt to improve the measurement of \( Q \) and the limits on \( m(\nu_e) \). The purpose of this letter is to develop the theory of the calorimetric spectrum in \(^{163}\text{Ho}\) decay, and to ascertain its sensitivity to the mass of the neutrino.

We proceed to analyze the spectrum of calorimetric energy \( E_c \) in the process

\[ ^{163}\text{Ho} \rightarrow \nu_e (E_\nu) + ^{163}\text{Dy}^H \rightarrow \nu_e (E_\nu) + ^{163}\text{Dy} + E_c \]  
(4a)

Here \( H \) labels the hole left in the daughter atom by electron capture. Capture is only allowed from \( H = nS \) and \( H = np_{1/2} \) orbitals, that have non-vanishing wave functions at the origin. Let \( E_H \) be the (positive) ionization energy of the \( H \) orbital. The \( Q \) values quoted in Eqs. (3) are such that \( E_L > Q > E_M \); capture is only allowed for \( n > 2 \), and \( H = M_1, M_2, N_1, N_2, \ldots \). The recoil energy of the \( \text{Dy} \) atoms in Eqs. (4) is completely negligible \((<2 \times 10^{-5} \text{ eV})\) so that \( Q = E_\nu + E_c \); the calorimetric spectrum is a measure of the neutrino energy spectrum. The \( E_c (E_\nu) \) spectrum consists of a series of peaks at \( E_c = E_H (E_\nu = Q - E_H) \) with relative weights given by ratios of wave functions at the origin \( \Psi_H^2(0) \). The peaks have Breit-Wigner shapes with the natural widths \( \Gamma_H \) of excited \( \text{Dy}^H \). The simplest way to understand the calorimetric spectrum \( dW/dE_c \) may be to use \( E_c = Q - E_\nu \), and to think of it as the neutrino spectrum \( dW/dE_\nu \) in the two-body process Eq. (4a), with the neutrino recoiling against a series of states with non-zero widths. This is almost all that need be said to write the spectrum:

\[
\frac{dW}{dE_c} = \mathcal{N} \sum_H \left\{ (Q - E_c) \sqrt{(Q - E_c)^2 - m_{\nu}^2} \right\} \Gamma_H/2 \pi \left( \frac{E_c - E_H}{2} + \frac{\Gamma_H^2}{4} \right) 
\]  
(5)
and its integral, which in an excellent narrow width approximation is:

$$W = \mathcal{N} \sum_H \mathcal{Y}_H^2(\phi) (Q - E_H) \sqrt{(Q - E_H)^2 - m_y^2} \quad (6)$$

The constant $\mathcal{N}$ drops from the normalized spectrum $dW/dE_C$ of interest to us, and contains the squares of the nuclear matrix element and Fermi coupling strength. The phase space factor in curly brackets in Eq. (5) is nothing but $E_y|\mathbf{p}_y|^2$. The $^{147}$Tb atom decays predominantly by electron de-excitations (Coster-Kronig and Auger transitions): the calculated fluorescence yields are $^81 \omega(M_1) = 1.1 \times 10^{-3}$, $\omega(M_2) = 1.6 \times 10^{-3}$, $\omega(N_1) = 3.7 \times 10^{-5}$, $\omega(N_2) = 7.0 \times 10^{-5}$. The Breit-Wigner shapes in Eq. (5) would have been affected by an electron momentum factor $p_e$ from phase space in the dominant $^{147}$Tb electron decays, if not because, at these very low energies, $p_e = \sqrt{\epsilon/c}$ is precisely compensated by the Coulomb attraction correction. Finally, Eqs. (5) and (6) are "classical" in that we have neglected interferences between intermediate states with the same quantum numbers (i.e., $H = M_1, N_1, O_1, \ldots$) decaying into the same final states; and we have neglected the virtual contributions of $H = K, L$ states. We proceed to give qualitative and quantitative arguments why the "non-classical" corrections are negligible. The $H = K, L$ states in Eq. (4a) lie well above $E_C(\text{max}) = Q$, and are suppressed by large energy denominators. The dominant de-excitations of $H = nS, nP_{1/2}$; $n > 2$ states are Coster-Kronig transitions, $H = H'\text{He}^-$, with one of the final holes in an orbital with the same original $n$ [i.e., $\Gamma$(Coster-Kronig)/$\Gamma$(Auger) = 16.6, 8.5, 166, 129; for $M_{1,2}, N_{1,2}$ holes, respectively $^81$]. Thus, $(nS, n^S)$ and $(nP_{1/2}, n^P_{1/2})$; $n \neq n'$ interferences between different intermediate states in Eq. (4a) are unlikely, because their decay products tend to be different. We have used the transition matrix elements computed by McGuire $^8$ to estimate that the neglected "non-classical" corrections are much smaller than 0.3% (0.1%) at the dominant $N_1(M_1)$ peaks of the spectrum and are at most at the per cent level at the endpoint $E_C \approx Q$. The effect of these corrections on the shape of the spectrum a few tens of eV from the endpoint is entirely negligible.

The full line of Fig. 1a displays $dW/dE_C$ from Eqs. (5) and (6); for $Q = 2.58$ keV, as in Eqs. (3a) and $N_y = 0$. The dashed line in Fig. 1a is the same spectrum smoothed with detector resolution, assumed to be a Gaussian with full width at half maximum $FWHM = 100$ eV. The $M_1(2.047$ keV) and $M_2(1.842$ keV) peaks would still be visible with this resolution, but the $N_1(0.416$ keV) and $N_2(0.332$ keV) peaks merge into one. The $O_1(0.063$ keV) and $O_2(0.026$ keV) peaks and a $P_1$ peak (too narrow to be shown in the figures) become a broad low-energy enhancement. Figure 1b shows two smoothed spectra, both with
FWHM = 100 eV for Q = 2.58 keV, as in Eq. (3a) and Q = 2.3 keV, as in Eq. (3b). Notice that the ratios between M and N peaks are very sensitive to Q, a fact to be exploited below. The parameters used in these plots are ratios of wave functions at the origin in Ho (Z = 67) and full widths of excited states of Dy (Z = 66). Several calculations of the first set of parameters exist in the literature, and they are quoted in Table 1. The spread between different calculations is generally at the 5% level and would not be very visible in Fig. 1 (except for the O peaks). The widths we have used for the Dy states are those calculated by McGuire: \( \Gamma(M_1) = 18 \) eV, \( \Gamma(M_2) = 10 \) eV, \( \Gamma(N_1) = 15 \) eV, \( \Gamma(N_2) = 11 \) eV. For illustrative purposes, we have adopted the guesses \( \Gamma(O_1) = 9 \) eV, \( \Gamma(O_2) = 2 \) eV (the properties of O levels will not affect the physics of interest to us). In a perfect resolution spectrum the widths of the levels would of course play a role and be in fact measurable. Clearly, the sensitivity to the assumed values of \( \Gamma_H \) in an experiment with coarse resolution (FWHM \( \ll \Gamma_H \)) is very small.

<table>
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<th>Reference</th>
<th>9)</th>
<th>10)</th>
<th>11)</th>
<th>12)</th>
<th>13)</th>
<th>14)</th>
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<td>( N_1/M_1 )</td>
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<td>0.241</td>
<td>0.242</td>
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<tr>
<td>( M_2/M_1 )</td>
<td>0.0532</td>
<td>0.0542</td>
<td>0.0551</td>
<td>0.0552</td>
<td>0.0543</td>
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<tr>
<td>( O_2/O_1 )</td>
<td>0.05 (our guess estimate, only for illustrative purposes)</td>
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Table 1

Ratios of squared wave function at the nucleus, for Z = 67. References 12) and 13) are non-relativistic calculations. The atomic potentials are Hartree-Fock in Refs. 9) and 12); Hartree-Fock-Slater in Refs. 10), 11) and 13); and Thomas-Fermi-Dirac in Refs. 14) and 15).
In Fig. 2 we illustrate a very efficient method to determine \( Q(\text{Ho}, \text{Dy}) \) in calorimetric experiments. What are shown are ratios of peak heights as functions of \( Q \), as predicted by Eq. (5), convoluted with our assumed Gaussian energy resolution, FWHM = 100 eV. Figure 2a shows the ratio of the \( M_1 \) peak to the \( N_{1,2} \) peak and Fig. 2b the ratio \( M_1/M_2 \). The dashed regions are for \( m(\nu_e) = 0 \) and their width reflects the spread between the different theoretical calculations of wave function ratios (see Table 1). The ratio \( M_1/N \) is much more sensitive to \( Q \) than the ratio \( M_1/M_2 \), since the \( Q \) value is much closer to the \( M \) binding energies than to the \( N \) ones. The dashed lines are for \( m(\nu_e) = 60 \) eV and the wave function ratios of Mann and Weber9). \( Q \) and \( m_\nu \) could, in principle, be extracted from a simultaneous measurement of the \( M_1/N \) and \( M_1/M_2 \) ratios, but, as the figure illustrates, the sensitivity to a non-zero neutrino mass is only relevant if \( Q < 2.2 \) keV or if the wave function ratios could be determined with high precision either theoretically or experimentally. The ratios of peak heights can be measured with very high statistics. Suppose one arbitrarily takes the spread of computations of wave function ratios (Table 1) to be a measure of theoretical uncertainty. Then, Fig. 2 implies that \( Q \) can be measured with a theoretical uncertainty of the order of \( \pm 10 \) eV (\( \pm 5 \) eV) if \( Q \) is in the neighbourhood of 2.58 keV (2.30 keV).

We finally come to the subject of neutrino mass effects near the endpoint \( E_c \sim Q \). The first crucial question is one of counting rate. Define a figure of merit \( g \) as the fraction of events in the interval \( Q - m_\nu, Q \) in the normalized spectrum \( dW(m_\nu = 0)/dE_c \) of Eqs. (5) and (6).

\[
g(Q, m_\nu) = \frac{1}{W(Q)} \int_{Q - m_\nu}^{Q} dE_c \frac{dW(Q, m_\nu = 0)}{dE_c}
\]

This is a good measure of the difference in fractional counting rates for \( m_\nu = 0, m_\nu \neq 0 \). The figure of merit in \( ^9\text{B} \) decay is \( g \sim 8 \times 10^{-3} (m_\nu/30 \text{ eV})^3 \). The figure of merit for \( \text{Ho} \) decay is not quite cubic in neutrino mass, particularly for very low \( Q \) values, since the Breit-Wigner matrix element affects the spectral shape. The \( \text{Ho} \) figures of merit, for a set of representative \( Q \) values\(^6\),\(^7\), are given in Table 2.
<table>
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<tr>
<th>Q(keV)</th>
<th>2.15</th>
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<th>2.48</th>
<th>2.58</th>
<th>2.68</th>
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<td>(g(Q, \nu = 30 \text{ eV}))</td>
<td>(4.5 \times 10^{-6})</td>
<td>(4.4 \times 10^{-7})</td>
<td>(1.1 \times 10^{-7})</td>
<td>(6.1 \times 10^{-8})</td>
<td>(3.7 \times 10^{-8})</td>
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<td>(g(Q, \nu = 60 \text{ eV}))</td>
<td>(7.4 \times 10^{-5})</td>
<td>(4.4 \times 10^{-6})</td>
<td>(9.7 \times 10^{-7})</td>
<td>(5.3 \times 10^{-7})</td>
<td>(3.2 \times 10^{-7})</td>
</tr>
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</table>

Table 2

Ho figures of merit, from Eqs. (5)-(7)

Notice that the figures of merit in Ho decay are superior to those in \(^3\text{H}\) decay. From this point of view, and for \(\nu \approx 30 \text{ eV}\) and \(Q = 2.58\), as in Eq. (3a) Ho is superior to \(^3\text{H}\) by an order of magnitude; for \(Q = 2.30\), as in Eq. (3b), Ho is superior to \(^3\text{H}\) by a factor of \(\approx 50\). If the implantation of Ho into a solid state detector is as successful as the implantation of \(^3\text{H}\), this is good news.

In Fig. 3 we have displayed the traditional "Kurie" plots: \((dW/\mathrm{d}E_c)^{1/2}\) versus \(E_c\). Figure 3a is for perfect resolution; in Fig. 3b theory is convoluted with a Gaussian with FWHM = 100 eV. Both figures show curves for \(\nu = 0.60 \text{ eV}\) and \(Q = 2.3, 2.58 \text{ keV}\). Since the Q value can, in principle, be determined with high precision from the peak ratios discussed before, and the figures of merit are favourable, it is not excluded that an electron neutrino mass at the 30 eV level can be detected in this kind of experiment. It need not be emphasized that here, resolution is the main concern. Since \(Q(\text{Ho}) << Q(^3\text{H})\), the final word on resolution, one way or another, may not have been said\(^5\).

A limiting factor of calorimetric experiments is "pileup": two single events can accidentally occur within the same time resolution window, and register the sum of their energies. The time resolution, \(\Delta t\), is limited below by the charge collection time, of the order of 6us in Simpson's\(^5\) relatively huge detector (80mm\(^2\) x 5mm). Let \(N\) and \(T_{1/2}\) be the number and half-life of \(^{161}\text{Ho}\) atoms. The fraction of accidental double coincidences per single event is \(N \Delta t \ln 2 / T_{1/2}\). The energy spectrum of accidentals, normalized in the same way, is:

\[
\frac{d\mathcal{A}}{dE_c} = \frac{N \Delta t \ln 2}{T_{1/2}} \frac{1}{a} \frac{d\alpha}{dE_c}
\]

\[
\frac{1}{a} \frac{d\alpha}{dE_c} = \frac{1}{W^2} \int dE_1, dE_2 \frac{dW}{dE_1} \frac{dW}{dE_2} \mathcal{S}(E_c - E_1 - E_2)
\]
with \( \frac{dW}{dE} \) the single spectrum of Eqs. (5) and (6). In Fig. 4a we show \( \frac{da}{dE} \) for \( Q = 2.58 \text{ keV} \), both with ideal resolution and smoothed with a Gaussian (FWHM = 100 eV). Figure 4b is a comparison of smoothed spectra for \( Q = 2.58 \text{ keV} \) and 2.3 keV. The pile-up spectrum peaks at \( E_C = E_R + E_{\gamma} \), with \( H = M_1, N_{1,1,1}, 0_{1,1,1} \) (the \( P_1 \) contribution is negligible). For the \( Q \) values of Eqs. (3), the endpoint of singles spectrum is close to the \( M+N \) peaks of the doubles spectrum. To illustrate the relevance of accidentals, we compute the number of atoms \( N(Q) \) for which single and accidental events are equally numerous in the region sensitive to the neutrino mass. For an experiment with FWHM > \( m_\nu \) (but not much bigger) one can see from Fig. 3b that the \( m_\nu \) sensitive region roughly extends from \( Q = 2(\text{FWHM}) \) to \( Q + \text{FWHM} \). For \( \Delta t = 1 \text{us} \) and FWHM = 100 eV, \( N(Q = 2.58 \text{ keV}) = 6.8 \times 10^{13} \) and \( N(Q = 2.3 \text{ keV}) = 6.1 \times 10^{15} \), a huge number. The number of single events in this \( m_\nu \) sensitive region would be \( 2.5 \times 10^5 \) per year at \( Q = 2.58 \text{ keV} \), and \( 3.1 \times 10^9 \) per year at \( Q = 2.3 \text{ keV} \). With the use of the figures of merit of Table 2, we conclude that the first number of events/year is barely enough to see the effect of \( m_\nu = 60 \text{ eV} \), while the second number is more than enough to measure \( m_\nu = 30 \text{ eV} \). The limitation for the unfavourable \( Q \) values (close to a large accidental peak) may be much less serious than it sounds, since the accidental background can be computed from the observed singles spectrum and/or measured with great accuracy by artificially increasing the time gate \( \Delta t \) and/or tamed with other pile-up rejection methods.

To summarize, an assured outcome of an \( \text{Ho}^\text{163} \) calorimeter experiment would be a very good and very welcome determination of the \( (\text{Ho,Dy}) Q \) value, or, more precisely, the ratios of phase space factors \( \frac{n(Q - E_H)(Q - E_H)^2 - m_\nu^2}{} \) for \( H = M_1, N_2 \) and \( N \) levels. Because of atomic physics uncertainties, these ratios are convincingly sensitive to a \( \approx 30 \text{ eV} \) neutrino mass only for \( Q \) values in the lower range of the KKK experiment. The endpoint of the Ho decay spectrum is resonance-enhanced by its proximity to the \( M_1 \) binding energy. Consequently, and for a Ho calorimeter detector performing in all respects as well as Simpson’s Tritium detector, the favourable figure of merit would make the endpoint analysis superior for Holmium than for Tritium. This statement must be qualified by the limitation implied by accidental coincidences, a violently varying function of time resolution, experimental ingenuity and plain good luck (the precise value of \( Q \)). We believe that this kind of experiment should be given one or more tries.

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FIGURE CAPTIONS

Fig. 1 : Normalized energy spectra for m_v = 0.

Fig. 2 : Ratio of peak heights with Gaussian resolution (FWHM = 100 eV), for
        m_v = 0 and m_v = 60 eV.

Fig. 3 : "Kurie" plots near to the spectral endpoint.

Fig. 4 : "File-up" normalized spectra of double accidental coincidences.
Fig. 1

(a) $Q = 2.58$ keV

- **Ideal Resolution**
- **FWHM = 100 eV**

(b) $Q = 2.58$ keV

- **Q = 2.30 keV**
- **FWHM = 100 eV**

Fig. 1
\begin{center}
\textbf{Fig. 3}
\end{center}
Fig. 4