SINGLE ELECTRON EJECTION IN ELECTRON CAPTURE AS A TOOL
TO MEASURE THE ELECTRON NEUTRINO MASS

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ABSTRACT

The electron capture decay $^{163}\text{Ho} \rightarrow ^{163}\text{Dy}^{\text{H}} + \nu_e$ occurs with a record low energy release, $Q \sim 2.6$ keV. The daughter Dy^{H} atom has an electron hole, H, and predominantly decays by electron ejection $\text{Dy}^{\text{H}} \rightarrow \text{Dy}^{\text{H}_1\text{H}_2} + e^-$. We investigate the neutrino mass sensitivity of the electron spectrum in the over-all process $\text{Ho} \rightarrow \text{Dy}^{\text{H}_1\text{H}_2} + e^- + \nu_e$. In this spectrum, the fraction of events sensitive to a fixed non-zero neutrino mass is one to two orders of magnitude smaller than in the standard case of tritium β -decay. But the electron energies in ^{163}Ho decay are considerably smaller than in ^3H decay ($Q \sim 18$ keV). This suggests experiments whose energy resolution could be much better than that of the magnetic spectrometers conventionally used in the tritium case.

1. - INTRODUCTION AND OUTLOOK

The most stringent experimental limits on the electron antineutrino mass

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

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

$$14 \text{ eV} < m(\tilde{\nu}_e) < 46 \text{ eV} \quad (99\% \text{ conf.}) \quad [\text{Lubimov et al.}^3]$$

result from the analysis of the spectral endpoint shape⁴⁾ in tritium β -decay. The only experiment that claims a lower limit³⁾ on $m(\bar{\nu}_e)$ measures the electron momentum with a magnetic spectrometer. Its quoted resolution³⁾ is 45 eV at the m_ν sensitive endpoint energies: $E_{\max}^e \lesssim Q \equiv M(^3\text{H}) - M(^3\text{He}^+) \approx 18.6$ keV. Tritium is the substance of choice because of its relatively short half-life ($T_{1/2} \sim 12$ years) and small Q value. The smaller the electron energies, the better the absolute momentum measurements. The smaller the Q value, the larger the fraction of events that are sensitive to a given neutrino mass. Only an isotope, ^{187}Re , is known⁵⁾ to β -decay with a smaller energy release than ^3H . Should the ^{187}Re lifetime not be disappointingly long ($T_{1/2} \sim 4 \cdot 10^{10}$ years), neutrino mass hunters would presumably be irresistibly tempted by its record-small energy release: $Q(^{187}\text{Re}, ^{187}\text{Os}^+) \sim 2.6$ keV⁵⁾. Comparably small Q values, in m_ν sensitive processes with much shorter lifetimes, can be found amongst weak electron capture decays. In this paper we discuss the best known candidate: ^{163}Ho .

^{163}Ho decays by electron capture into ^{163}Dy and an electron neutrino. The nucleus of the daughter Dy is left in its ground state, but the Dy atom is unstable: it has a hole, H, in the orbital from which the electron is captured. The Dy^{H} atom is obviously neutral, having an extra electron "misplaced" (relative to stable atomic Dy) in the weakly bound $\text{N}_7(4f_{7/2})$ level where its residence used to be, in ^{163}Ho . Let Q denote the mass difference between the ground state ^{163}Ho and ^{163}Dy atoms, and let E_{H} be the (positive) ionization energy of the H level in Dy. The available (neutrino) energy in the capture process turns out to be so small that only capture from M_1 and more external orbitals is allowed ($E_{\text{K}}, E_{\text{L}} > Q > E_{\text{M}}$).

The half-life and Q value in ^{163}Ho decay have recently been measured by observing the Dy M-X-ray and M-Auger electrons, from sources with a known number of ^{163}Ho atoms, in the chain processes

with $H = M$ in Eq. (1.1a). The results are:

$$Q = 2.58 \pm 0.10 \text{ keV} ; T_{1/2} = (7 \pm 3) \text{ years} \quad [\text{Andersen et al.}^{6)}] \quad (1.2a)$$

$$Q = 2.30 \pm 0.15 \text{ keV} ; T_{1/2} = 900^{+500}_{-200} \text{ years} \quad [\text{Yasumi et al.}^{7)}] \quad (1.2b)$$

The difference between the quoted values does not seem to originate in a discrepancy in the observed M capture half-life, but from differences in the nuclear matrix elements employed to extract a Q value and a total half-life^{*}).

Only electrons whose wave function at the origin $\phi(0)$ does not vanish [$j = 1/2$; $H = nS$, $nP_{1/2} = M_{1,2}, N_{1,2}, O_{1,2}, P_1$] may interact with the nucleus and contribute to the capture process of Eq. (1.1a). For a given n , the contribution of the S ($L = 0$) electrons dominate, the non-vanishing of $\phi^2[nP_{1/2}]$ at the origin being a relativistic correction at the few per cent level.

Consider the chain of Eqs. (1.1a) and (1.1b) as a single three-body process

Here the star in the intermediate state is meant to emphasize that it need not be precisely on-shell: its mass is uncertain by the width of the unstable Dy^H state. The photon spectrum is not a superposition of strictly monochromatic lines, but extends all the way to the kinematically allowed limit of the three-body process. The sensitivity^{4),8)} of the photon spectrum $d\omega^{H'}/dk$ to a non-zero neutrino mass is maximal at the endpoint of the spectrum ($k \rightarrow k_{\text{max}} \sim Q - E_{H'}$), where a massive neutrino may be emitted "at rest". For a conveniently chosen H' ($4P_{1/2}, 4P_{3/2}, 5P_{1/2}, 5P_{3/2}$) $d\omega^{H'}/dk$ has prominent X-ray resonances. The dominant ones close to the endpoint correspond to an intermediate state $H = M_1$, have energies $k_{\text{res}} = E(M_1) - E(H')$, and lie below k_{max} at a distance $Q - E(M_1) = \text{few hundred eV}$ ($E_{M_1}(\text{Dy}) = 2.047 \text{ keV}$). The X-ray widths are of order $\sim 10 \text{ eV}$ and their effect at the spectral endpoint can still be felt as an enormous enhancement of the photon yield⁸⁾. In other words, the matrix element for the process of Eq. (1.3) is enhanced and dominated at $k \approx k_{\text{max}}$ by the close-by pole at $k = k_{\text{res}}$. Since the fraction of events that are sensitive to $m_\nu \neq 0$ is generally small, this may be good news.

A limitation of single particle endpoint measurements, well documented in tritium β -decay⁹⁾, concerns the fact that the daughter atom can be left in a variety of different states with different masses. The spectral endpoint is

* The values in Eqs. (1) and (2) are extracted from electron capture decay rates under the assumption that $(Q - E(M_1))^2 \gg m_\nu^2$. The best direct Q value measurement, from nuclear reaction kinematics⁶⁾, gives the result $Q = 2.3 \pm 1.0 \text{ keV}$.

a superposition of branches ending at differential energies. This problem is particularly acute if, as is the case for past tritium experiments, the resolution is comparable or larger than the spread between the endpoints of different decay branches. In atomic tritium the main decay branches⁹⁾ are to the ground state of He^+ (70% probability) and its first excited level at ~ 41 eV (25% probability).

An advantage of "bremmstrahlung" photon measurements in processes like the one of Eq. (1.3), is that it may be possible to overcome the aforementioned complications at the spectral endpoint. The photon spectrum can be measured in coincidence with Auger (or Coster-Kronig) electron lines

The electron signs the H' hole, serves to disentangle the different decay branches, and allows one to study single branch spectral endpoints. Coincidence experiments aimed at constraining the electron neutrino mass, and checking the theory of electron capture in isotopes where K capture is forbidden, have been performed with ^{193}Pt as the source of activity¹⁰⁾. They give a limit $m(\nu_e) < 500$ eV, an order of magnitude improvement over previous electron neutrino (as opposed to antineutrino) measurements¹¹⁾. Similar experiments with a ^{163}Ho source are in preparation.

Consider next, the chain of Eqs. (1.1a)-(1.1c) as a single three-body process

This process and its potential as a tool to measure $m(\nu_e)$ are the subject of this paper. We refer to the reaction Eq. (5) as SEEEC, for *single electron ejection in electron capture*. Most of what we said about the photon emission process of Eq. (1.3) can be repeated, mutatis mutandis, for SEEEC. All one has to do is substitute X-rays for Auger lines, X-ray tails for Auger tails, and photon spectral endpoints for ejected electron spectral endpoints. The endpoint in the process of Eq. (5), for $m_\nu = 0$, is at an electron kinetic energy

$$E_{\max} = Q - E(H_1, H_2) \approx Q - E(H_1) - E(H_2) \quad (1.6)$$

Close to the endpoint from below, there will be prominent Auger lines, the dominant ones resulting from M_1 capture, and having energies

$$E_{\text{res}} = E(M_1) - E(H_1, H_2) \approx E(M_1) - E(H_1) - E(H_2) \quad (1.7)$$

These resonances lie below the corresponding endpoints at the same distance as in the photon process $E_{\text{max}} - E_{\text{res}} \approx Q - E(M_1) \sim$ few hundred eV. Their effect at the endpoint is to enhance the spectrum in the m_ν sensitive region by several orders of magnitude, relative to the expectation in a typical K-capturing isotope, say ^{55}Fe , in which the atomic resonances lie well below the spectral endpoint.

The main limitation of a neutrino mass search in SEEEC is the same as in tritium β -decay: in a measurement of a single ejected electron the state (H_1, H_2) of the daughter atom is left unspecified^{*)}. This implies that the electron spectral endpoint is a complicated superposition of different branches, corresponding to the different possibilities for H_1 and H_2 . We shall argue that, given enough statistics, the effects of a non-vanishing neutrino mass at the few eV level may still be visible, in spite of the many-branch problem. Three reasons underlie this assertion:

- i) electrons with a maximal energy of ~ 2.6 keV can be measured (perhaps by electrostatic rather than electromagnetic means) with a resolution at the eV level or beyond;
- ii) two effects may modify the shape of the electron spectrum at the endpoint, relative to a simple, one-channel, $m_\nu = 0$, expectation (a straight Kurie plot). One is the superposition of different channels with different endpoints. This makes the spectrum (or its square root: the Kurie plot) tend towards zero more gently than the naïve expectation. The other effect is a possible non-vanishing neutrino mass. This makes the spectrum bend towards zero at the different endpoints more abruptly than in the naïve expectation. The two effects can be visibly disentangled if the uncertainty due to a limited resolution is smaller than the spread between the different dominant endpoints. This level of resolution has not been achieved in past tritium experiments;

^{*)} Experiments where three electrons are observed, two of them providing the signature for the holes H_1, H_2 , can be contemplated¹²⁾. They are clearly much harder than SEEEC experiments, and presumably to be relegated to a "second generation".

iii) the theoretical expectation for the shape of the SEEEC endpoint is fairly complicated. It involves, among other parameters, branching ratios for Auger transitions that have not been measured experimentally. An experiment that is, from the point of view of statistics, sensitive to a few eV neutrino mass would have enormous statistics at the peaks of the Auger lines. The parameters most relevant to the endpoint analysis can therefore be determined with precision where the statistics is bound to be large.

In Chapter 2 we outline theoretical expectations for the shape of the SEEEC spectrum in ^{163}Ho decay at all energies but the ones very close to the endpoint. We expect a fiendishly complicated spectrum, dominated by a very large number of electron ejection resonances. In Chapter 3 we analyze the spectral endpoint in detail and its sensitivity to a non-zero neutrino mass. The spectral endpoint is dominated by the tails of a few resonances, and is a superposition of decays into a few dominant $\text{Dy}^{H_1 H_2}$ states with H_1, H_2 corresponding to very weakly bound electrons. We argue that neutrino mass effects for $m_\nu \lesssim 10$ eV should be visible in the spectrum, in spite of considerable theoretical uncertainties and all sorts of atomic complications. A particular problem, the shake-off or shake-up of spectator electrons, is treated in detail in an Appendix, and found to be irrelevant, unlike in tritium decay. The crucial question of rate is discussed in Chapter 4. We find that the production of the source activity necessary for an experiment that competes in endpoint statistics with the tritium experiments¹⁾⁻³⁾ is not a limitation. But if the source is a monoatomic layer, it would be geometrically large. It is not easy to compare different experimental approaches, some of which have not been tried. We attempt to do it in Chapter 5.

2. - THE SPECTRUM OF EJECTED ELECTRONS IN ^{163}Ho DECAY

In this chapter we compute the electron energy spectrum in the process

$$^{163}\text{Ho} \rightarrow X + e^-(E) + \nu_e \quad (2.1)$$

where the notation "X" is meant to emphasize that only a single electron of energy E is being observed. The state X may be the dysprosium atom with two holes; $\text{Dy}^{H_1 H_2}$, as in Eq. (1.5), or Dy with three vacancies plus an extra (unobserved) electron, etc. We proceed to discuss the electron spectrum in the process Eq. (2.1), at energies not very close to the endpoint. The detailed discussion of the spectral endpoint shape is relegated to the subsequent chapter.

Consider first the single electron ejection process $X = \text{Dy}^{H_1 H_2}$ in Eq. (2.1). The leading $O(G\alpha)$ diagrams for this process are shown in Fig. 1a and 1b, where the continuous lines labelled 1 and 2 refer to the electrons being captured and ejected, and the dotted lines labelled $H_{1,2}$ are the corresponding vacancies in the daughter Dy atom. The dashed lines are Coulomb interactions. We proceed to study the process in an approximation where electrons are treated as moving independently in the Coulomb field of the nucleus. This is only to identify and discuss the main (resonant) contributions that will eventually be computed in a more realistic fashion. Let $\phi_{1,2}^e$ and ϕ_f^e be the electron wave functions in the Coulomb field of the nucleus with Z protons. We work in the non-relativistic approximation for capture from nS orbitals, and to first order in v/c for capture from $nP_{1/2}$ orbitals. Since the $\text{Ho} \rightarrow \text{Dy}$ nuclear transition is of the "allowed, unhindered" type⁶⁾, the wave functions of the captured electrons can, in our approximation, be substituted by their values at the origin $\phi(0)$. The matrix element for the process under consideration can be written as¹³⁾:

$$M = -\alpha \frac{G}{\sqrt{2}} \frac{1-P_{12}}{\sqrt{2}} \Phi^\nu(0) \mathcal{N} \int d\vec{r}_1 d\vec{r}_2 G_{\bar{E}}(0, \vec{r}_1) \phi_1^e(\vec{r}_1) \phi_f^e(\vec{r}_2) \phi_2^e(\vec{r}_2) \left(\frac{1}{r_2} - \frac{1}{r_{12}} \right) \quad (2.2)$$

where P_{12} is the two-electron exchange operator, $r_2 = |\vec{r}_2|$, $r_{12} = |\vec{r}_1 - \vec{r}_2|$, and $\mathcal{N}$ is the weak current nuclear matrix element, contracted with the leptonic current operator

$$\mathcal{N} = \langle Z-1 | J_\mu \gamma^\mu (1+\gamma_5) | Z \rangle \quad (2.3)$$

In Eq. (2.2) $G_{\bar{E}}$ is the electron propagator in the Coulomb field of the nucleus

$$G_{\bar{E}}(0, \vec{r}) = \sum_H \frac{\phi_H^e(0) \phi_H^e(\vec{r})}{\bar{E} + E_H} \quad (2.4)$$

where the wave functions are again Coulombic and the sum over H runs through bound and continuous $H = nS$ and $nP_{1/2}$ states of (positive) energy E_H . The term proportional to $1/r_2$ in Eq. (2.2) corresponds to the diagram of Fig. 1a, and reflects the effect on an expectant electron of the sudden change of nuclear charge: $Z \rightarrow Z - 1$. Following the treatment of Intemann and Pollock¹³⁾, we have developed the Coulombic wave functions $\phi(Z-1)$ in terms of $\phi(Z)$ plus $O(\alpha)$ corrections, to write the amplitude of Fig. 1a in the same form as the amplitude of Fig. 1b, which is more obviously of $O(\alpha)$, and corresponds to the term proportional to $1/r_{12}$ in Eq. (2.2).

The energy $\bar{E}$ in the propagator of Eq. (2.4) is the one flowing through the electron line of the captured electron in Figs. 1a and 1b. Let E be the energy of the ejected electron and let $E(H)$, $E(H_{1,2})$ be the (positive) ionization energies of the corresponding electronic levels. Energy conservation implies that the energy denominator in Eq. (2.4) can be rewritten as

$$\bar{E} + E_H = E_R - E \quad (2.5a)$$

$$E_R \equiv E(H) - E(H_1) - E(H_2) \quad (2.5b)$$

Whenever it is positive, E_R is the energy of an electron ejection line. The amplitude corresponding to the diagram of Fig. 1b is proportional to

$$M_b(H_1 H_2) \sim \sum_H \frac{\phi_H^e(0)}{E - E_R + i\Gamma/2} \int \frac{d\vec{r}_1 d\vec{r}_2}{r_{12}} \phi_H^e(\vec{r}_1) \phi_1^e(\vec{r}_1) \phi_f^e(\vec{r}_2) \phi_2^e(\vec{r}_2) \quad (2.6)$$

where we have given to the state H its natural width. Written in the form of Eq. (2.6), the amplitude M_b is recognizable as the product of a capture amplitude ($\sim \phi_H^e(0)$), the propagator of an unstable atomic state with a hole in the H orbital (the energy denominator) and the Coulomb amplitude for an electron ejection transition $H \rightarrow H_1 H_2 e_f$ (the integral). It is to this possibly resonant amplitude that we have referred in the introduction, when "classically" discussing electron ejection as a two-step process, see Eq. (1.5) and the ensuing discussion. In the form of Eq. (2.6) the M_b amplitude of Fig. 1b is more readily interpretable as corresponding to the differently time ordered diagram of Fig. 1c or, in a more compact notation, the one of Fig. 1d. The possibly resonant character of M_b is crystal-clear in these diagrams. The existence of this other time-ordering compensates for the fact that we had apparently "forgotten" the exclusion principle in letting the propagator in Eq. (2.4) run over states that, in the atom, may already be occupied.

The amplitude corresponding to Fig. 1a is proportional to

$$M_a(H_1 H_2) \sim (1 - P_{12}) \frac{\phi_H^e(0)}{\bar{E} + E_H} \int d\vec{r}_1 \phi_a^e(\vec{r}_1) \phi_1^e(\vec{r}_1) \int \frac{d\vec{r}_2}{r_2} \phi_f^e(\vec{r}_2) \phi_2^e(r_2) = \quad (2.7)$$

$$= (1 - P_{12}) \frac{\phi_{\alpha}^e(0)}{E + E(H_2)} \int_{\alpha_1} \frac{d\vec{r}_2}{r_2} \phi_f^e(\vec{r}_2) \phi_z^e(\vec{r}_2) \quad (2.7) \text{ cont.}$$

and is non-vanishing only if one of the final holes $H_{1,2}$ is in an orbital from which direct capture may occur ($\delta_{\alpha 1} \neq 0$, $H_1 = nS, nP_{1/2}$). This term in the total amplitude is never resonant ($E + E(H_2) > 0$). We neglect it in the rest of this discussion since (except for the endpoint, the subject of next chapter) we are only interested in the single spectrum close to the resonant energies where the spectrum is large and the non-resonant background negligible. We shall see that the density of resonances is so high, that the endpoint region is the only few hundred eV long energy domain with no resonances in it.

Now that we have approximated the electron ejection amplitude by the resonant expression Eq. (2.6), we can proceed to write, and explain, a simple expression for the normalized single electron spectrum of Eq. (2.1). The spectrum is a sum of resonances with Breit-Wigner shapes, weighted with the branching ratios $\beta(H; H_1, H_2)$ for the different transitions, and with the probability P_H of capture resulting in a vacancy in the H orbital:

$$\frac{1}{W} \frac{dW}{dE} \approx \sum_{H, H_1, H_2} P_H \beta \frac{\Gamma/2\pi}{(E - E_R)^2 + \Gamma^2/4} \quad (2.8)$$

Here, P_H , β , E_R and Γ are functions of the intermediate and final holes H and $H_{1,2}$. The quantities $E_R(H, H_1, H_2)$ are the energies of electron ejection lines, as given by Eqs. (2.5b). In the real resonance approximation only those E_R such that $0 < E_R < Q$, are kept. The quantities $\Gamma_R(H, H_1, H_2)$ in Eq. (2.8) are the natural widths of the corresponding lines. $\beta(H, H_1, H_2)$ is the branching ratio for the transition $Dy^H \rightarrow Dy^{H_1 H_2} + e^-$. In ^{163}Ho , electron capture is only possible for $H = M$, or more external orbitals. The fluorescence yield ω (fractional probability for X-ray emission) from such orbitals is tiny^{*}). Thus

$$\sum_{H, H_2} \beta(H; H_1, H_2) \approx 1 \quad (2.9)$$

^{*}) According to the calculations of McGuire¹⁴⁾ $\omega(M_1) = 1.1 \cdot 10^{-3}$, $\omega(M_2) = 1.8 \cdot 10^{-3}$, $\omega(N_1) = 3.7 \cdot 10^{-5}$, $\omega(N_2) = 7 \cdot 10^{-5}$.

Let $\alpha(H)$ be the fractional electron capture probability from the H orbital, proportional to the square of electron wave function at the origin and to the available phase space. In the $m_V^2 \ll (Q - E_H)^2$ approximation:

$$\alpha(H) = \frac{|\psi_H(0)|^2 (Q - E_H)^2}{\sum_{H'} |\psi_{H'}(0)|^2 (Q - E_{H'})^2} \quad (2.10a)$$

$$\sum_H \alpha(H) = 1 \quad (2.10b)$$

Should we be considering the electron spectrum for $X = Dy^{H_1 H_2}$ in Eq. (2.1), the quantity P in Eq. (2.8) would be $P = \alpha(H)$ and the corresponding energy spectrum, normalized as in Eq. (2.8) to the total capture probability, would (approximately) integrate to unity. But in an "inclusive" experiment that detects only single electrons, these need not be first generation ones. The Dy^H atom de-excites by a series of electron emission processes, all of which contribute to the single electron spectrum. Thus, the quantity P_H in Eq. (2.8) is the sum of a direct capture contribution, and cascade contributions in which the H vacancy is due to capture in a deeper than H level, followed by electron ejection processes producing an H hole:

$$P_H = \alpha(H) + \sum_{l,m} \alpha(l) \beta(l; H, m) c_1 + \sum_{l,m,n,r} \alpha(l) \beta(l; m, n) \beta(m; H, r) c_2 + \dots \quad (2.11)$$

Here, c_i are conditional functions taking care of the finite electron population in the different atomic levels. Their explicit form is cumbersome, of interest only to logicians, and their effect in practice is not large: we will not discuss them further.

Before presenting actual results based on Eq. (2.8), we pause for a few more comments. The integral $\bar{W}/W$ of the inclusive electron spectrum is the average electron multiplicity $n > 1$. The electron momentum in electron phase space ($p^2 dp \sim p m_e dE$) does not appear in Eq. (2.8), since, at the very low energies relevant to Ho decay, it is a very good approximation to cancel it against the Coulomb attraction correction. Satellization effects have been

ignored: we do not know how to correct electron transition energies and branching ratios by the effect of possibly having extra vacancies in the electron-ejecting Dy atom. Equation (2.8) is "classical", in the sense that we have neglected quantum interference effects, the effects of the tails of virtual resonances, and the contribution of the continuum of unbound electron energies in the captured electron propagator. None of these effects are important close to prominent resonances in the spectrum: everywhere but in the endpoint region. We shall reconsider all neglected effects when discussing the spectral endpoint, the only region sensitive to neutrino masses, where we need to understand the shape of the spectrum with more precision.

To illustrate the prediction of Eq. (2.8) we have used the ratios of electron wave functions calculated by Mann and Waber¹⁵⁾ and reproduced in Table 1, and the electron widths and branching ratios extensively computed by Mc Guire¹⁴⁾. Both of these calculations go well beyond the Coulombic approximation that we have used to identify the main resonant contributions. Mann and Waber¹⁵⁾ use a relativistic Hartree-Fock approach. McGuire approximates the central potential of Herman and Skillman¹⁶⁾ in order to compute the single electron wave functions used to estimate electron ejection rates and fluorescence yields. The binding energies and total widths in the calculations are reproduced in Table 2. Some levels ($O_{2,3}$, $N_{4,5}$, $N_{6,7}$) are listed as degenerate. There should even be some "multiple splitting" within these and other levels. due to unfilled $4f$ ($N_{6,7}$) shells. We come back to fine questions of structure when discussing the spectral endpoint in the next chapter. The single electron spectrum is shown in Fig. 2, for $Q = 2.58$ keV, the central value quoted⁶⁾ in Eq. (1.2a). The most prominent transitions are labelled by $(H, H_1 H_2)$. Most of the gorgeous structure of this spectrum, and even the question of whether the complicated theoretical atomic physics that underlies the prediction is precise or not, are not crucial to neutrino mass measurements. The actual spectrum, if ever measured with a resolution at the eV level, may differ quite a bit from that of Fig. 2. For one thing, we have not split the $O_{2,3}$, $N_{4,5}$ and $N_{6,7}$ levels and we have neglected satellization and multiplet splitting effects: the saw is bound to have more teeth. Moreover most peaks in the spectrum, but those at the highest energies, result from the de-excitation of holes that can be formed in a variety of complicated cascades: errors in theoretical branching ratios are bound to be cumulative, see Eq. (2.11).

When discussing neutrino mass effects at the spectral endpoint in the next chapter, we shall see that the transition matrix element is dominated by the tails of a few prominent resonances that lie close to the endpoint. We shall argue that neutrino mass effects may be visible "to the naked eye" in the spectral

shape, independently of the precise values of the parameters that determine the size of the matrix elements. But knowledge of the parameters of the higher energy resonances, particularly their energy spacings and relative prominence, can only help. The three most prominent highest energy resonances in Fig. 2 are the $M_1 \rightarrow N_{4,5} N_{6,7}; O_1 N_{6,7}$ and $N_{6,7} N_{6,7}$ lines. Other resonances in this energy domain ($M_1 \rightarrow P_1 P_1; N_{6,7} P_1; O_{2,3} N_{6,7}; O_{2,3} O_{2,3}; O_1 O_{2,3}; O_1 O_1; N_{4,5} P_1$) do not show in the spectrum: their branching ratios as computed by McGuire are too small. All of these closest-to-the-endpoint resonances are transitions from the deepest capturing level: M_1 . Vacancies on M_1 can only be made by direct capture, not by cascade transitions from deeper levels. Measurement of the widths and relative heights of the resonances directly yield the parameters (widths, energies and branching ratios) most relevant to the extrapolation of the matrix element to the endpoint of the spectrum.

H	$ \phi_H(0)/\phi_{M_1}(0) ^2$	$\alpha(H)$
M_1	1	0.17
M_2	0.053	0.018
N_1	0.233	0.65
N_2	0.012	0.036
O_1	0.031	0.12
O_2	~ 0.001	0.006

Table 1 : Ratio of wave functions at the nucleus and capture probabilities for $Q = 2.58$ keV

H	$E_H(\text{keV})$	$\Gamma_H(\text{eV})$
K (1S)	53.79	[30]
L_1 (2S)	9.046	[5.91]
L_2 (2P $_{1/2}$)	8.581	[4.95]
L_3 (2P $_{3/2}$)	7.790	[3.90]
M_1 (3S)	2.047	18.3
M_2 (3P $_{1/2}$)	1.842	10.4
M_3 (3P $_{3/2}$)	1.676	10.2
M_4 (3D $_{3/2}$)	1.332	2.41
M_5 (3D $_{5/2}$)	1.295	1.38
N_1 (4S)	0.416	14.8
N_2 (4P $_{1/2}$)	0.332	11.2
N_3 (4P $_{3/2}$)	0.293	9.9
$N_{4,5}$ (4D $_{3/2,5/2}$)	0.154	4.35
O_1 (5S)	0.063	(9)
$O_{2,3}$ (5P $_{1/2,3/2}$)	0.026	(2)
$N_{6,7}$ (4F $_{5/2,7/2}$)	0.004	
P_1 (6S)	~0.002	

Table 2: Binding energies of Dy energy levels¹⁷⁾ and total width¹⁴⁾. Numbers in square brackets are not used in our calculations. The O_1 widths are a guess, used only for illustration purposes, as in Fig. 12.

3. - THE SPECTRAL ENDPOINT

The SEEEC decay of Ho:

is a three-body decay process, like β -decay. The sensitivity of the electron spectrum to a neutrino mass is the usual one⁴⁾, governed by neutrino phase space ($\sim E_\nu p_\nu$):

$$\begin{aligned} dW(H_1, H_2) / dE &\propto |\mathcal{M}(H_1, H_2)|^2 E_\nu p_\nu = \\ &= |\mathcal{M}(H_1, H_2)|^2 (E_{\text{end}} - E) \sqrt{(E_{\text{end}} - E)^2 - m_\nu^2} \end{aligned} \quad (3.2a)$$

$$E_{\text{end}}(H_1, H_2) \simeq Q - E(H_1) - E(H_2) \quad (3.2b)$$

where $\mathcal{M}(H_1, H_2)$ is the transition matrix element. Observation of the shape of the spectral endpoint limits or determines the neutrino mass⁴⁾. This simple statement must be qualified in practice by consideration of the following complications:

- i) in a single electron experiment, the identity of the daughter (H_1, H_2) state is unspecified, and the total spectrum is a superposition over different channels with different endpoint energies;
- ii) the description of the final dysprosium ion in Eq. (3.1) in terms of states with two holes is incomplete, for it is possible for the daughter ion to have more vacancies, or electrons that have moved to unoccupied orbitals. We devote an Appendix to argue that, unlike in tritium β -decay, this particular kind of "atomic interplay" problem does not have a serious incidence on m_ν measurements at the few eV level in ^{163}Ho decay.
- iii) when the energies of the daughter atom vacancies, $E(H_{1,2})$, are to be specified with precision at the few eV level, several complications arise. One of them is that the outer orbitals are affected by chemical and surface effects. Another complication is that in rare earths with unfilled $N_{6,7}$ ^(4f)

orbitals, the electronic levels within these and other orbitals suffer a "multiplet splitting", beyond the fine structure one;

- iv) the daughter $\text{Dy}^{H_1 H_2}$ atom is in an unstable state, its mass is not entirely well defined, and the endpoint energies Eqs. (3.2b) do not have sharp values.
- v) the matrix elements in Eq. (3.2a), unlike in low Q allowed β -decays, are not approximately constant. They are dominated by nearby resonances, that lie some 500 eV below the endpoint and have widths of order 10 eV;
- vi) knowledge of the resonant parameters (widths and branching ratios) is not enough to determine the matrix elements appearing in Eq. (3.2a). This is because of possible quantum interferences between different intermediate states in channels with the same final state. Moreover, in a single electron experiment, not all of the resonant parameters can be determined by measurements at the resonant energies, because of multiple electron ejection cascade effects;
- vii) we are unable to develop a precise theory of all the aforementioned complications, in spite of the fact that it is nothing more than an exercise in quantum mechanics.

Surprisingly enough, we proceed to argue that neutrino mass effects at the few eV level should be observable in the SEEEC Ho decay spectrum, in spite of all of the above complications. To preview this claim, we compare in Fig. 3 the shapes of the Kurie plots in two cases. One of them, labelled $M_1 \rightarrow N_{6,7} N_{6,7}$, is an oversimplified situation with only one capturing level and one final state, and none of the complications listed above. The other case, labelled "exact" in Fig. 3, is an example with reasonable estimates of all the complicated effects, to be discussed in more detail below. The spectral shape in the "exact" and the oversimplified situation are very similar, as the figures show for $m_\nu = 0$ and $m_\nu = 60$ eV. Two main reasons underlie the survival of neutrino mass effects from under the rubble of fiendishly complicated atomic physics. The first is that in the last tens of electron volts of the spectrum, the phase space factor is much more rapidly varying than the matrix element, in spite of the nearby resonances. The second reason is: of all the very many channels with endpoints in the last couple of hundred eV of the spectrum, only a minority have relatively large branching ratios.

We proceed to discuss the endpoint SEEEC spectrum with allowance for the complications listed above. In so doing we are handicapped by the fact that we have scarce experimental information on the widths and electron ejection branching ratios in Dy, particularly for the M levels. We heavily rely in what follows on theoretical calculations of these parameters by McGuire¹⁴⁾. The details of

our results should only be regarded as indicative, since the process of electron ejection from outer orbitals is a deviously complicated one, and McGuire's widths are known in certain cases to be overestimates¹⁸⁾. As we shall see, confidence on the detailed expectation for the endpoint shape can be gained as the experiment itself constrains the relevant parameters.

The electron energy domain of direct interest to neutrino mass measurements encompasses not only the top-most few hundred eV's of the spectrum, but also the region of the most energetic M_1 capture dominated resonances, $E \gtrsim 1.85$ keV, see Fig. 2. The tails of these nearby resonances dominate the matrix element at the endpoint energies. To be specific, we define a "high energy domain" as the whole range of interest: $1.85 \text{ keV} \lesssim E \lesssim Q$. We define as the "endpoint region" a subset of the high energy domain: the top-most ~ 150 eV of the spectrum. The analysis that follows is supposed to describe the whole high energy domain.

All of the very many $(H_1 H_2)$ channels for which $E(H_1) + E(H_2) \lesssim 150$ eV have endpoints $E_{\text{end}}(H_1 H_2)$ in the endpoint region, see Eq. (3.2b). The precise location of the ultimate endpoint, $\max\{E_{\text{end}}\}$, is less relevant to the search of neutrino mass effects than the distance between the endpoints of channels whose branching ratios are large. With McGuire's branching ratios, the dominant channels in the endpoint region are tails of the last few prominent resonances in Fig. 2: $H_1 H_2 = N_{6,7} N_{6,7}, N_{4,5} N_{6,7}$ and, to a lesser extent, $O_1 N_{6,7}$. The dominance of these channels is to a large extent just an electron multiplicity effect, no doubt qualitatively correct. In Table 3, we list the endpoint energies as distances to the top-most dominant channel: $E(H_1 H_2) - E(N_{6,7} N_{6,7})$. Also given in the table are McGuire's branching ratios to be used in the following discussion.

Some levels that should be split by fine structure effects of a few eV, like O_2 and O_3 , are listed in Table 3 as degenerate, due to lack of electron capture data. More important is the fact that in atoms with incomplete $N_{6,7}$ orbitals, the corresponding levels and even other levels suffer a "multiplet splitting", that gives them a fairly complicated structure at the few eV level. These splittings have been observed in X-ray induced electron ejection experiments (X.P.S.: X-ray photo-electron spectroscopy) on rare earths, and are known to depend on the chemical state of the atom¹⁹⁾. Electron capture experiments sufficiently precise to observe these effects have not been performed, and the level population of X.P.S. experiments cannot directly be translated into expectations for e-capture processes. Moreover, we do not know how to compute with confidence any of these complicated effects. We will rely below on the oft-emphasized fact that the level spacings and branching ratios for the dominant M_1 mediated transitions should be precisely measurable at the resonant energies. We shall also investigate with some examples how multiplet splitting may affect the endpoint analysis.

$H_1 H_2$	$P_1 P_1$	$N_{6,7} P_1$	$N_{6,7} N_{6,7}$	$O_{2,3} P_1$	$O_{2,3} N_{6,7}$	$O_{2,3} O_{2,3}$	$O_1 P_1$	$O_1 N_{6,7}$	$O_1 O_{2,3}$	$O_1 O_1$	$N_{4,5} P_1$	$N_{4,5} N_{6,7}$	$N_{4,5} O_{2,3}$
$E(H_1 H_2) - E(N_{6,7} N_{6,7})$	?	- 2 eV	0	20 eV	22 eV	44 eV	57 eV	59 eV	81 eV	118 eV	148 eV	150 eV	172 eV
$\beta[M_1 \rightarrow H_1 H_2]$	$9 \cdot 10^{-7}$	$8 \cdot 10^{-5}$	$3 \cdot 10^{-3}$	10^{-5}	10^{-4}	10^{-5}	$7 \cdot 10^{-6}$	$7 \cdot 10^{-4}$	10^{-4}	$5 \cdot 10^{-5}$	$2 \cdot 10^{-4}$	$7 \cdot 10^{-3}$	$2 \cdot 10^{-4}$
$\beta[N_1 \rightarrow H_1 H_2]$	$9 \cdot 10^{-6}$	$2 \cdot 10^{-3}$	$2 \cdot 10^{-2}$	$3 \cdot 10^{-4}$	10^{-2}	10^{-3}	$2 \cdot 10^{-4}$	$2 \cdot 10^{-2}$	$3 \cdot 10^{-3}$	10^{-3}	$5 \cdot 10^{-3}$	$7 \cdot 10^{-2}$	$2 \cdot 10^{-2}$
$\beta[M_2 \rightarrow H_1 H_2]$	$8 \cdot 10^{-8}$	$8 \cdot 10^{-6}$	$8 \cdot 10^{-3}$	10^{-5}	$2 \cdot 10^{-3}$	$2 \cdot 10^{-4}$	$2 \cdot 10^{-6}$	$6 \cdot 10^{-5}$	$8 \cdot 10^{-5}$	$5 \cdot 10^{-6}$	$2 \cdot 10^{-5}$	$5 \cdot 10^{-3}$	$3 \cdot 10^{-3}$

Table 3: Energies¹⁷⁾ and branching ratios¹⁴⁾ relevant to the endpoint analysis.

We proceed to discuss the SEEEC spectrum in the high energy domain, in the "classical" resonant approximation. This means that we momentarily neglect interference effects, and the non-resonant backgrounds of Eq. (2.7). In the high energy domain, the several electron cascade effects reflected in Eq. (2.11) are negligible, and strictly absent for the M_1 mediated contributions that are resonant and dominant at these energies. The SEEEC spectrum is a sum of resonances, each one directly weighted with a capture probability $\alpha(H)$, a branching ratio $\beta(H \rightarrow H_1 H_2)$ and the appropriate phase space factors:

$$\frac{1}{W} \frac{dW}{dE} = \sum_{H, H_1, H_2} \frac{\alpha(H) \beta(H \rightarrow H_1 H_2)}{(Q-E_H) \sqrt{(Q-E_H)^2 - m_\nu^2}} \int_0^{Q-E-m_\nu} dE' \mathcal{L}_1 \mathcal{L}_2 (Q-E-E') \sqrt{(Q-E-E')^2 - m_\nu^2}$$

$$\mathcal{L}_1 \equiv \mathcal{L}(E+E'; E_H; \Gamma_H) \quad (3.4)$$

$$\mathcal{L}_2 \equiv \mathcal{L}(E'; E(H_1 H_2); \Gamma(H_1) + \Gamma(H_2))$$

$$\mathcal{L}(a, b, \gamma) \equiv \frac{1}{2\pi} \frac{\gamma}{(a-b)^2 + \gamma^2/4}$$

where all the quantities have been previously defined. The Lorentzian factors $\mathcal{L}$ take into account the non-zero widths of parent and daughter Dy states. The phase space factor under the integral sign reflects the fact that the mass of the final state is uncertain, $\Gamma(H_1) + \Gamma(H_2) \neq 0$. The phase space factor at a resonant energy in the denominator is purely for normalization. Close to a particular resonance $M_1 \rightarrow H_1 H_2$, Eq. (3.4) reduces to an expression of the form of Eq. (2.8):

$$\left. \frac{1}{W} \frac{dW}{dE} \right|_{E \sim E_R} \simeq \alpha(M_1) \beta(M_1; H_1 H_2) \mathcal{L}(E; E_R; \Gamma) \quad (3.5a)$$

$$E_R \simeq E(M_1) - E(H_1) - E(H_2) \quad (3.5b)$$

$$\Gamma \simeq \Gamma(M_1) + \Gamma(H_1) + \Gamma(H_2) \quad (3.5c)$$

A fit of Eqs. (3.5) to the experimentally observed resonances would determine the resonant energies, relative branching ratios and widths. Moreover, the resonant structure in the high energy domain, if measured with the required resolution, would show the multiplet splitting that may be relevant to the endpoint analysis, and self-consistently determine the necessary parameters: energy splittings and relative branching ratios. All we are saying is that allowance for these effects must be made in Eqs. (3.4) and (3.5). This fixes the parameters that play a dominant role in the extrapolation of the matrix element to the endpoint. The parameters that cannot be so easily extricated from the spectrum itself are the ones governing the interference effects to be discussed below and the parameters describing the tails of resonances $H = M_2, N_{1,2}, O_{1,2}$ that lie further from the endpoint [the number of events under these resonances is not directly proportional to a capture branching ratio, but reflects multiple electron transitions, as in Eq. (2.11)]. These parameters describe relatively small contributions to the matrix elements, the bulk of which is described by the M_1 transition contributions. Variation of these parameters within reasonable limits changes the over-all magnitude of the spectrum in the endpoint region, but does not obliterate the sensitivity to $m_\nu \neq 0$ of the spectral endpoint shape.

We proceed to discuss numerical expectations for the endpoint spectrum. With branching ratios as given in Table 3, the channels $H_1H_2 = N_{6,7}N_{6,7}, O_1N_{6,7}$ and $N_{4,5}N_{6,7}$ dominate the high energy domain and the endpoint region itself. This reflects their relatively large $\beta(M_1)$ branching ratios. Some other branching ratios from N_1 and M_2 intermediate states are also relatively large, but their contribution to the spectrum of Eq. (3.4) is small. The N_1 contributions are damped near the endpoint by relatively large energy denominators: $Q - E(N_1) \approx 2.16$ keV, $Q - E(M_1) \approx 0.53$ keV, for Q as in Eq. (2.2a). The M_2 contributions are damped by the relatively small capture probability from $P_{1/2}$ levels. The N_1 contributions have an effect on the over-all magnitude of the spectral endpoint bigger than what the "classical" resonant formula, Eq. (3.4), would seem to imply. This is because the final state quantum numbers in $M_1 \rightarrow H_1H_2e^-$ and $N_1 \rightarrow H_1H_2e^-$ transitions are the same, giving rise to interference between the corresponding matrix elements. We have studied this effect on the three dominant H_1H_2 channels by use of the matrix elements, rather than the transition rates, computed by McGuire. The effect of interferences is undramatic, in the sense that they cannot conceivably imitate neutrino mass effects. All they do, in the example where we use McGuire's parameters, is to reduce the counting rate in the last 200 eV of the spectrum by a smooth factor that varies between 0.9 and 0.75 in this relatively large interval.

In Fig. 4 we show the normalized spectrum dW/WdE in the endpoint region, for $Q = 2.58$ keV, and $m_\nu = 0$ (Fig. 4a), $m_\nu = 60$ eV (Fig. 4b). The curves are computed for the parameters given in Tables 2 and 3, with allowance for the interference effects that we just discussed. Multiplet splitting effects have not yet been taken into account. Channels other than the three whose contributions are explicitly shown in the figure are small and very slowly varying in this energy domain. The figure, when looked at with sufficient concentration, shows the usual sensitivity to $m_\nu \neq 0$ in the endpoint shape. Everything is as if there was only one dominant channel $H_1 H_2 = N_{6,7} N_{6,7}$, in the sense that $m_\nu \neq 0$ effects on the total spectrum are very small at the endpoint energies of the $O_1 N_{6,7}$ and $N_{4,5} N_{6,7}$ channels. Thus the qualitative statement that one channel is dominant in the last few hundred eV of the spectrum suffices to give a fair prediction of the m_ν sensitivity of its shape^{*)}. Neutrino mass effects are more apparent to the naked eye in the Kurie plot. Figure 5b shows the Kurie plot translation of Fig. 4, and compares the expectations for $m_\nu = 0, 30, 60$ eV. Figure 5a, in which $Q = 2.30$ keV as in Eq. (2.2b), dramatizes the sensitivity of the counting rate to the precise value of $Q - E(M_1)$.

We close our overview of the many complications of the spectral endpoint shape with a discussion of "multiplet splitting" effects. The most relevant splitting neglected so far concerns the substructure of the $N_{6,7}$ channels that we have seen to be dominant in the region of the spectrum sensitive to neutrino masses at the few eV level. Holmium and dysprosium are rare earths with incomplete $N_{6,7}$ ($4f_{5/2,7/2}$) shells. In the free atomic state, Ho has 11 and Dy has 10 $4f$ electrons. Both metallic Ho and the stable Dy^+ ion have seven spin "up" and three spin "down" $4f$ electrons, with their energy levels distant by some ~ 5 eV. The structure or "multiplet splitting" of these incomplete shells is more complicated than a mere fine splitting. X-ray photoelectron experiments have shown that the spin "up" and "down" levels have a substructure consisting in two to four narrow lines spaced by 2 or 3 eV. To make matters more complicated, the whole structure of the $4f$ level is dependent on the chemical state of the sample (i.e., whether it is metallic or oxidized). Once again, we are unable to outline a theory of these effects, and the experiment will eventually have to rely on the observation of multiplet splitting - if it is prominent and thus relevant - as a structure within the $M_1 \rightarrow N_{6,7} N_{6,7}$ peak in the electron ejection spectrum. To develop a feeling for the possible incidence of multiplet splitting effects on the shape of the spectral endpoint we have given

^{*)} This is clearly satisfactory, particularly in view of the fact that we have not treated the $O_1 N_{6,7}$ contribution with as much loving care as the others. For this channel the non-resonant amplitude of Eq. (2.7) does not vanish. Its effect is to reduce the $O_1 N_{6,7}$ contribution, perhaps by as much as 50 %.

the $N_{6,7}$ levels, a substructure that approximates the observed one in Dy. The $N_{6,7}$ level is split into two components, a narrow one ($\Gamma \sim 1$ eV) for the spin "down" electrons and a broad one ($\Gamma \sim 4$ eV) centered at a 5 eV higher binding energy and approximating the two or three narrow, closely spaced, spin "up" levels. We have estimated the M_1 branching ratios into pairs of electrons in these levels by mere combinatorics, based on the fact that there are seven electrons in the spin up level and three in the spin down one. In Fig. 6 we compare the endpoint shapes of the Kurie plot for $m_\nu = 0, 30, 60$ eV in two cases. The full lines correspond to our explicit example with multiplet splitting. The dotted lines correspond to the case discussed before, with the $N_{6,7}$ levels all degenerate and having a binding energy that coincides with the "baricentre" of the split case. The figure indicates that the effects of $m_\nu > 0(10 \text{ eV})$ would still be visible to the naked eye (and all the more to an actual fit to the spectral shape) in spite of multiplet splitting at the few eV level.

To summarize, we have considered in this section all the effects we know could complicate the analysis of the SEEEC endpoint shape. The main problem, as in tritium decay, is the multiplicity of decay channels with endpoints spaced by $0(10 \text{ eV})$. In an extreme case where there would be, say, one hundred different channels with equal branching ratios and endpoints spaced by 1 eV, the effects of an assumed m_ν of 30 eV would not be visible in a spectrum that sums over all these channels. If the explicit estimates we have made are not extreme oversimplifications, a few channels should be relevant at the endpoint and the above mentioned extreme case should be very unrealistic. Given sufficient statistics and its possibly high resolution, a search for neutrino masses in SEEEC Ho decay may well compete with the classical ^3H experiments.

4. - THE QUESTION OF RATE

To compare the fraction of decays sensitive to a non-zero neutrino mass in different processes, it is useful to introduce a rough measure of the fraction of decay events lying in the region of the spectrum whose shape is "visibly" m_ν dependent. The simplest such "figure of merit" is

$$g(m_\nu) = \frac{1}{W} \int_{E_{\max} - m_\nu}^{E_{\max}} dE \frac{dW(m_\nu=0)}{dE} \quad (4.1)$$

a measure of the number of events "missing" at the spectral endpoint for $m_\nu \neq 0$. The figure of merit for tritium β -decay is

$$g(^3\text{H}, m_\nu) \simeq 1.9 \beta(n'=1) \left(\frac{m_\nu}{Q} \right)^3 \quad (4.2)$$

where $\beta(n' = 1)$ is the branching ratio for the decay into the He^+ ground state, $Q = 18.6$ keV and the over-all factor reflects Coulomb corrections. For $m_\nu = 30$ eV, $g(^3\text{H}) \sim 56 \cdot 10^{-10}$. The expression for, and the Q dependence of, the figure of merit in ^{163}Ho SEECC is not as simple as Eq. (4.2), due to the resonant enhancement close to the endpoint, but its numerical value is calculable from Eq. (3.4). In doing the calculation we take E_{max} to correspond to the endpoint of the dominant channel at the endpoint, $H_1 H_2 = N_{6,7} N_{6,7}$. The result for $Q = 2.58$ keV, as in Eq. (3.2a), and $m_\nu = 30$ eV is $g(\text{Ho}) = 10^{-10}$. This number increases by one order of magnitude for $Q = 2.3$ keV, as in Eq. (3.2b). In the rest of this chapter we use $m_\nu = 30$ eV in defining the "interesting events" and we set $Q = 2.58$ keV, the central experimental result for which the resonant enhancement is smallest. The figure of merit in inclusive or "calorimetric" experiments²⁰⁾ is larger for Ho than for ^3H ; the reduction in the Ho SEECC case being mainly due to the smallness of the calculated branching ratios $\beta(M_1 \rightarrow N_{6,7} N_{6,7})$, see Table 3.

Milligrams of ^{163}Ho can and have been person-made. With a half-life of 7 millenia, as in Eq. (1.2a), a milligram of ^{163}Ho would undergo $3.6 \cdot 10^{14}$ decays/year. Of these, $3.6 \cdot 10^4$ would be "interesting events". The fraction of these that would be transmitted through a hypothetical spectrometer with 0[few eV] resolution, we cannot tell. All we can say is that the spectrometer would not be of the take-home type, though its size would still be dwarfed by that of a typical high energy physics experiment. The point is that, to allow electrons to exit unhindered, the source would presumably have to consist of a monoatomic layer of ^{163}Ho resting on a backing. A monoatomic, one milligram, circular spot of Ho has a radius of the order of one foot.

5. - CONCLUSIONS

Limiting, or measuring, the electron neutrino mass at the few eV level is a task whose interest need not be emphasized. Indications³⁾ of a large (~ 35 eV) non-zero result contribute to make the task more timely. In the past, efforts concentrated on tritium decay (that measures the electron antineutrino mass),

double β -decay (relevant if the distinction between neutrino and antineutrino is only semantic) and neutrino oscillations (that rely on the hope of relatively large mixing angles). Exploration of other avenues is of interest. The fact that electron capture processes measure the mass of what "officially" is a neutrino, adds some spice to their complementarity.

Past tritium spectrometer experiments were limited by a combination of physico-chemical complications and insufficient resolution. The spectral endpoint is a superposition of channels - well understood for an atomic tritium source - that affect the spectral shape in a way "opposite" to the effect of a non-zero neutrino mass. With a resolution larger than the neutrino mass and the spacing between the dominant channels, an $m_\nu \neq 0$ result can only result from a fit to experimental data in which the neutrino mass effect is invisible to the naked eye. In principle, there is nothing wrong with this, but a fear of uneasiness and of possibly overlooked systematic effects. Three ways out of the dilemma suggest themselves:

- i) to improve the resolution of tritium experiments and to use an atomic source or a variety of non-atomic ones;
- ii) to perform coincidence experiments with a signature for the particular decay branch;
- iii) to do "tritium-like" calorimetric²⁾ or spectrometer^{1),3)} experiments with sources with a lower Q value. This allows one to envisage the possibility that the resolution (maximum electron energy) could be better (smaller) than for ^3H .

In this paper we have investigated the third route in the example of ^{163}Ho SEEEC. We find that the multibranch problem at the spectral endpoint is theoretically much more involved than for atomic tritium, comparable in complication to the case of a molecular tritium source. But there are two advantages to ^{163}Ho , and a disadvantage. The first and oft emphasized advantage is that the energy of 1 - 3 keV electrons should be measurable with eV precision. Perhaps ^3H experiments can also be pushed to this level. This is likely to suffice - given enough statistics - to disentangle m_ν effects from multibranch effects. The second advantage is that the multibranch structure of the endpoint is to a large extent reflected in the structure of the prominent resonances close to the endpoint, where the statistics may be huge. There is no tritium analogue of this. The disadvantage is that the decay rate of ^{163}Ho and the figure of merit of ^{163}Ho SEEEC are smaller than the corresponding ^3H figures. Whether these disadvantages can be overcome without a sacrifice in resolution, is the challenge.

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APPENDIX - ELECTRON SHAKE-UP AND SHAKE-OFF

In Chapter 3 we have discussed the "high energy" region of the SEEEC spectrum in the approximation that the dominant decay channels are those for which the daughter atom is left with two vacancies: $Dy^{H_1H_2}$, as in Eq. (3.1). We devote this Appendix to the argument that this approximation is a very good one. The possibly competing channels are those in which the daughter atom is left in a state $Dy^{H_1H_2H_3}$, meaning that an extra electron originally in the H_3 orbital has been "shaken-off" the atom, or "shaken-up" to some external unoccupied level. The claim is that the contribution of these channels to the high energy region of the spectrum is negligible. We shall refer to the shake-up/shake-off processes simply as shake-up, whenever no distinction is necessary.

Three leading types of effects contribute to the shake-up process, the amplitudes for which are depicted in Fig. 7. It is understood that their amplitudes should be summed and then squared, but we shall argue that the individual squared amplitudes are small and therefore we can use a classical language for each of them, as if the "different processes" in Fig. 7 and the different electrons were distinguishable.

Figure 7a shows a resonance dominated cascade process in which $Dy^{H_1H_2}$, with H_1H_2 two of the shallow levels relevant to the endpoint analysis, subsequently decays into $Dy^{H_1H_2H_3}$ by the emission of a very low energy electron. This effect has in fact tacitly been taken into account in Eq. (3.4) and in our calculations: it is embodied in the non-zero width of the $Dy^{H_1H_2}$ state, and has the effect of smoothing the endpoint shape of the corresponding decay branch. Figure 7b shows a resonance dominated cascade process in which the observed high energy electron is the "second" one. With the second electron in the "high energy" domain, this process is damped by two large energy denominators, and is entirely negligible. Figure 7c shows in detail a "sudden" process, in which one of the electrons is shaken-up as a consequence of the abrupt charge redistribution in electron capture. The rest of the Appendix is devoted to a discussion of this process.

When a 3H atom β -decays, the nuclear charge changes from $Z = 1$ to $Z = 2$. The expectant electron has a 30% probability of being shaken-up by the large change in the nuclear field, and may end up in different levels spaced 0(10 eV) apart. Figure 7c depicts the electron capture analogue of the 3H shake-up problem. The only electrons that need concern us are the ones in outer levels ($O_{1,2,3}, N_{6,7}, P_1$), whose binding energies are small, and whose ejection may affect the endpoint analysis. Though we will make some quantitative estimates, a qualitative argument suffices to convince oneself of the smallness of the

shake-up problem in electron capture relative to ^3H decay. In a relatively large Z material, like Ho, electron capture results in a small $(1/Z)$ fractional change in nuclear charge. Moreover the "missing proton charge" is shielded by the missing electron charge: it is only the charge distribution that changes. Unlike in ^3H β -decay, the potential acting on the spectator electrons changes little in the decay process, and their shake-up rate is small.

A numerically trustable calculation of the probability that one or more of the outer electrons is shaken up (the complement of the probability that they all "stay") would be a titanic task, involving a very detailed knowledge of atomic wave functions and their overlaps. All we shall attempt to give is a very rough estimate allowing one to conclude that the outer electron shake-up probability is orders of magnitude below the level where it would become worrisome to our purposes. In the sudden approximation in which the electron capture process is instantaneous in the scale of orbital electron motions, the amplitude for no electrons to be shaken up is the overlap $\langle \psi | \psi' \rangle$ of the atomic wave functions "before and after". The "before" wave function is that of Ho, the "after" wave function is modified by the absence of the nuclear charge and that of the captured electron. Let $j = 0_1; 0_{2,3}; N_{6,7}; P_1$ label the external orbitals, and let n_j be the corresponding occupation number (2; 6; 11; 2, respectively). Let ψ_j be the single electron wave function in Ho, and let $\psi'_j(Z-1, i)$ be the single electron wave function in the atom with one less proton and one electron hole in the orbital of the captured electron, i . We estimate the order of magnitude of the probability P_i that all external electrons remain in place as i -capture suddenly occurs, as:

$$P_i = \prod_j |\langle \psi_j | \psi'_j(Z-1, i) \rangle|^{2n_j} \quad (\text{A.1})$$

This formula deserves the following criticisms and counter criticisms:

- i) a correct expression would involve not only diagonal (j,j) terms, as in Eq. (A.1), but also exchange terms between orbitals of the same parity and angular momentum. The only example of an exchange term between external orbitals is $\langle P_1 | 0'_1 \rangle \langle 0_1 | P'_1 \rangle$. These terms are formally of the same order $(1/Z^2)$ as the deviations of the diagonal terms from unity. Since we shall find that the shake-up probability $1 - P_i$ is comfortably negligible, we have not estimated exchange effects;
- ii) equation (A.1) ignores exchange terms between external and internal orbitals, i.e., $\langle K | P'_1 \rangle \langle P_1 | K' \rangle$. The counter criticism is as before;

iii) in stating that the shake-up probability is $1 - P_i$, and treating electrons independently, we have ignored the fact that many electron levels are occupied, and electrons cannot move to them. This goes in the safe direction of making our estimate of a shake-up probability an overestimate.

There exist in the literature computations of the Ho and Dy wave functions ψ_j relevant to our analysis, but not of the wave functions $\psi_j^i(\text{Dy}, i)$ of dysprosium with a missing electron in the i orbital and an extra electron in the $N_{6,7}$ orbital. We shall capitalize on the recent Hartree-Fock calculations of McLean and McLean²¹). It is sufficient for our purposes to use, not the explicit solutions of the Hartree-Fock calculations, but just Coulombic approximations to them, $\psi_j(Z_{\text{eff}})$, where Z_{eff} is chosen so as to reproduce the mean radius of the "exact" wave function. The objects of interest to us are overlaps of nearly identical wave functions, and even with use of sophisticated self-consistent calculations, only the order of magnitude of the deviations of these overlaps from unity is to be trusted. Just to check that the Coulombic approximation gives results of the same order of magnitude as the "exact" Hartree-Fock calculation, we give in Table 4 the comparison between $\langle \psi_j(\text{Ho}) | \psi_j(\text{Dy}) \rangle$ for Hartree-Fock wave functions and their respective effective charge Coulombic approximations. We proceed to define α_{ij} as the effective charge seen by the j electron due to the presence or absence of the captured i electron:

$$\alpha_{ij} \approx \int d\vec{r} d\vec{r}' |\psi_j(\vec{r})|^2 |\psi_i(\vec{r}')|^2 \theta(r-r') \quad (\text{A.2})$$

We estimate the "after capture" wave function ψ^i of Eq. (A.1) as

$$\psi_j^i(Z-1, i) \approx \psi_j(Z_{\text{eff}}(\text{Ho}) - 1 + \alpha_{ij}) \quad (\text{A.3})$$

This reflects the fact that the ψ_j^i electrons "see" one less proton charge plus the effective charge of the missing captured electron. To check whether this is a sensible procedure, we have studied the hypothetical case of a missing $i = N_{6,7}$ electron. In this case the wave function of Eq. (A.3) should be an estimate of a dysprosium wave function from a holmium wave function. Again, the "exact" and approximate overlaps $1 - \langle \text{Ho} | \text{Dy} \rangle$ coincide within a factor 2 to 3, good enough for our purposes.

j	O ₁	O _{2,3}	N _{6,7}	P ₁
$1 - \langle \psi_j(\text{Ho}) \psi_j(\text{Dy}) \rangle_{\text{HF}}$	$5.5 \cdot 10^{-4}$	$4.36 \cdot 10^{-4}$	$4.1 \cdot 10^{-4}$	$1.6 \cdot 10^{-4}$
$1 - \langle \psi_j(\text{Ho}, Z_{\text{eff}}) \psi_j(\text{Dy}, Z'_{\text{eff}}) \rangle$	$13.3 \cdot 10^{-4}$	$10.4 \cdot 10^{-4}$	$7.5 \cdot 10^{-4}$	$7.0 \cdot 10^{-4}$

Table 4: Hartree-Fock and Coulomb-like wave function overlaps

With the approximations described above, and for the M_1 capture process that dominates the high energy region of the spectrum, we find for the quantities relevant to Eq. (A.1) the values:

$$\begin{aligned}
 1 - \langle N_{6,7} | N'_{6,7}(Z-1, M_1) \rangle &= 3.1 \cdot 10^{-7} \\
 1 - \langle O_{2,3} | O'_{2,3}(Z-1, M_1) \rangle &= 4.8 \cdot 10^{-6} \\
 1 - \langle O_1 | O'_1(Z-1, M_1) \rangle &= 4.3 \cdot 10^{-6} \\
 1 - \langle P_1 | P'_1(Z-1, M_1) \rangle &= 8 \cdot 10^{-7}
 \end{aligned}$$

Upon insertion of the above expressions into Eq. (A.1), we find $1 - P_i \sim 8 \cdot 10^{-5}$ for $i = M_1$. The outer electron ejection probability for the process dominant at the endpoint is negligible. The same type of estimates for $1 - P_i$, $i = N_1$, O_1 capture give $4.7 \cdot 10^{-3}$ and 0.06. We have not made estimates for M_2 , N_2 and P_1 capture, since the corresponding capture probabilities are very small. The ejection probability in O_1 capture may be as large as 6%, but the corresponding capture probability is only at the 10% level. Moreover a large energy denominator damps the contribution of O_1 capture relative to M_1 capture at the endpoint of the spectrum. In M_1 capture the ejection probability is negligible and the case of N_1 capture is in between M_1 and O_1 . A 1% bound for the outer electron ejection probability in the endpoint region is certainly a safe one. In a Holmium compound, as opposed to atomic Holmium, an $N_{6,7}$ electron may be promoted to the O_4 orbital. We have also made estimates of shake-up probabilities in this configuration. The results are practically identical to the ones discussed above.

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FIGURE CAPTIONS

- Fig. 1 : a),b) Leading electron ejection diagrams in electron capture
c) A different time-ordering of diagram b)
d) Compact notation for diagram c).
- Fig. 2 : Calculated inclusive electron ejection spectrum in ^{163}Ho decay.
- Fig. 3 : Kurie plot of the SEEEC endpoint for $m_\nu = 0, 60$ eV. The continuous line takes into account the many decay branches and other complications described in text. The dashed line is a renormalized dominant channel approximation.
- Fig. 4 : Normalized SEEEC spectrum in the endpoint region for $m_\nu = 0$ (a) and 60 eV (b). Individual contributions of single important channels are shown as dashed lines.
- Fig. 5 : Kurie plots for the SEEEC spectral endpoint, for two Q values and $m_\nu = 0, 30, 60$ eV.
- Fig. 6 : Kurie plots of the SEEEC spectral endpoint for $Q = 2.58$ keV, $m_\nu = 0, 30, 60$ eV. Continuous (dotted) lines (do not) include an estimate of multiplet splitting effects.
- Fig. 7 : Three contributions to shake-up/shake-off effects. Diagrams a), b) describe cascade effects. Diagram c) corresponds to a "sudden" process.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6

Fig. 7