Improved description of one- and two-hole excitations after electron capture in ^{163}Ho and the determination of the neutrino mass

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The atomic pair ^{163}Ho and ^{163}Dy, because of its small Q value of about 2.5 keV, seems to be the best pair to use to determine the neutrino mass by electron capture. The bolometer spectrum measures the full deexcitation energy of dysprosium (by x rays and Auger electrons plus the recoil of holmium, which can be neglected). The spectrum has an upper limit given by the Q value minus the neutrino mass. Till now this spectrum has been calculated in dysprosium allowing excitations with $3s_{1/2}$, $3p_{1/2}$, $4s_{1/2}$, $4p_{1/2}$, $5s_{1/2}$, and $5p_{1/2}$ (and $6s_{1/2}$) holes only. Robertson [R. G. H. Robertson, arXiv:1411.2906v1] also recently calculated the spectrum with two-electron-hole excitations in Dy. He took the probability for the excitation for the second electron hole from the work of Carlson and Nestor [T. A. Carlson, C. W. Nestor, T. C. Tucker, and F. B. Malik, Phys. Rev. **169**, 27 (1968); T. A. Carlson and C. W. Nestor, Phys. Rev. A **8**, 2887 (1973)] for $Z = 54$ xenon. The neutrino mass must finally be obtained by a simultaneous fit of the Q value, together with the properties of the relevant resonances, and the neutrino mass to the the upper end of the spectrum. Under the assumption that only one resonance (independent of its nature: one-hole, two-hole, multihole, or of other origin) near the Q value determines the upper end of the spectrum and that the profile of this leading state is Lorentzian, one has to fit simultaneously four parameters (neutrino mass, strength, distance of the leading resonance to the Q value, and width). If more than one resonance is of comparable importance for the upper end of the spectrum, it might be difficult or even impossible to extract the neutrino mass reliably. Compared to the work of Robertson this work includes the following improvements. (i) The two-hole probabilities are calculated in the Dirac-Hartree-Fock (DHF) approach for holmium and dysprosium but not for xenon. (ii) In calculating the probability for the second electron hole in dysprosium the $ns_{1/2}$ or $np_{1/2}$ ($n \geqslant 3$) one-hole states are included self-consistently in the DHF iteration. (iii) Because dysprosium has $Z = 66$ electrons and xenon only has $Z = 54$ electrons, one has at least eight additional two-hole states that do not exist in xenon and thus their probabilities have not been calculated by Carlson and Nestor and have not been included by Robertson. They are included here. (iv) For the probabilities of the one-hole states, which determine the main structure of the spectrum, the overlap and exchange corrections are taken into account. (v) In solving the DHF electron wave functions the finite size of the nuclear charge distribution is included. (vi) The nuclear matrix elements for electron capture integrate the charge of the captured electron over the nucleus with the weight $\psi(r)^2_{e,n,\ell,j} r^2$. Thus, for the capture probability the value $\psi^2_{e,n,\ell,j}(R)R^2$ is taken at the nuclear radius and not the value $\psi^2_{e,n,\ell,j}(r = 0.0)$ at $r = 0.0$, which has the weight r^2 zero. (vii) The formulas are derived in second quantization including automatically the antisymmetrization.

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I. INTRODUCTION

The determination of the absolute value of the neutrino masses is one of the most important open problems in particle physics. Presently major efforts are under way to measure in single-β decay, specifically in tritium decay, the electron antineutrino mass (KATRIN) [1]. Neutrinoless double-β decay can distinguish between Dirac and Majorana neutrinos and is in principle able to measure the effective Majorana neutrino mass [2]. Electron capture measures the electron neutrino mass [3–6]. The sensitivity to the electron neutrino mass is increased (as in single-β decay) in electron capture by a smaller Q value. Perhaps the best system for the determination of the absolute scale of the electron neutrino mass (and with the help of neutrino oscillations also of the muon and tauon neutrinos) by electron capture is the system $^{163}_{67}$Ho and $^{163}_{66}$Dy.

The electron neutrino mass can in principle be determined by the upper end of the deexcitation (bolometer) spectrum of ^{163}Dy after electron capture in ^{163}Ho. All deexcitation spectra (x rays, Auger electrons, and the recoil of holmium) end at the Q value (for ^{163}Ho around 2.5 keV; see Sec. II for the present Q-value situation) minus the neutrino mass.

Recently Robertson [7] included in the atomic excitations of dysprosium a second hole. The deexcitation bolometer spectrum including the two-hole states adds to the leading contributions of the one-hole spectrum a "fine structure." For the probability of the second hole in $Z = 66$ Dy, Robertson used results of Carlson *et al.* [8] and Carlson and Nestor [9] determined in $Z = 54$ xenon.

The neutrino mass must be obtained by a simultaneous fit of the Q value and the neutrino mass to the upper end of the spectrum including also properties of one-hole, two-hole, and other excitations close to Q. This complicates the neutrino mass determination. In cases where several resonances determine the upper end of the spectrum this can make the determination of the neutrino mass even impossible. If only one resonance determines the upper end of the spectrum and the line profile is Lorentzian, one has to fit four parameters: neutrino mass, the distance of the leading resonance to the

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Q value, the strength, and the width. Before one fits the theoretical spectrum to the upper end of the measurement, one has to fold the detector response including the finite resolution into the theory.

The improvements compared to the work of Robertson [7], Carlson *et al.* [8], and Carlson and Nestor [9] are the following.

(i) The two-hole probabilities are calculated here with the fully relativistic Dirac-Hartree-Fock (DHF) code of Grant [10], Desclaux [11], and Ankudinov *et al.* [12] with full antisymmetrization in the atoms holmium and dysprosium involved in the electron capture and not in xenon.

(ii) In calculating the probability for the second electron hole in dysprosium the $ns_{1/2}$ or $np_{1/2}$ ($n \geqslant 3$) one-hole states are included self-consistently in the DHF iteration. Thus for each one-hole state in dysprosium a full self-consistent DHF iteration with a hole in the different one-hole states is performed for all electrons in the atom. The electron wave functions in Ho and Dy for the same quantum numbers $|n,\ell,j\rangle$ but with different holes change markedly. In a very rough approximation for a first orientation without the Pauli correction the probability for the second hole is

$$P(\text{two-hole}) \approx [1.0 - \langle \text{Ho},n,\ell,j|\text{Dy},n,\ell,j\rangle^{2(2j+1)}]. \quad (1)$$

The overlap of electron orbitals with the same quantum numbers in Ho and Dy is typically around 0.999 [see Eqs. (2) and (3)]. Thus a relative change in the overlap by 1% can change the two-hole probability by a factor of 10. Equation (1) serves as a lever to enlarge a small change or error in the overlap into a large change in the two-hole probability. Therefore the electron wave functions for the overlaps should be calculated in holmium and dysprosium, and in the determination of the Dy electron wave functions the one-hole state must be self-consistently included if one wants to obtain reliable probabilities for the two-hole states.

(iii) Because in $Z = 66$ dysprosium there are more electrons than in $Z = 54$ xenon, there are at least eight additional two-hole states ($3s_{1/2}\ 4f_{5/2}$; $3s_{1/2}\ 4f_{7/2}$; $3p_{1/2}\ 4f_{5/2}$; $3p_{1/2}\ 4f_{7/2}$; $4s_{1/2}\ 4f_{5/2}$; $4s_{1/2}\ 4f_{7/2}$; $4p_{1/2}\ 4f_{5/2}$; $4p_{1/2}\ 4f_{7/2}$), which do not exist in xenon, and thus their probabilities have not been calculated by Carlson *et al.* [8] and Carlson and Nestor [9]and have not been included by Robertson [7]. They are included here. The excitation energies of these states are, according to Tables I and II, around 2050, 1845, 415, and 335 eV. Two-hole states involving the one-hole orbital $6s_{1/2}$ ($P1$) are not included here, because already the $5s_{1/2}$ orbital has an excitation energy of only 44.7 eV. The $6s_{1/2}$ excitation energy is expected to be around 5 eV, i.e., 100 times smaller than the excitations neglected by Robertson [7]. In addition the ionization energy of the $6s_{1/2}$ state in the atoms involved seems not to be available in the literature and these very lightly bound electrons are not well described by Slater determinants due to configuration mixing.

(iv) The electron wave functions in the parent atom and in the daughter atom get more and more similar with increasing charge number Z, because the relative change $\Delta Z/Z$ is smaller. Thus the overlaps of the wave functions for Z in the parent and $(Z-1)$ in the daughter increase closer to unity and the sudden approximation yields a smaller two-hole excitation probability, which is very roughly given by Eq. (1). The overlaps are tabulated in Faessler *et al.* [4]. They are close to unity. Thus the change of these

TABLE I. One- and two-hole states in ^{163}Dy with quantum numbers n, ℓ, and j. E_C is the excitation energy of the one- and the two-hole states. We adopt here for a better comparison of the values for E_c and the width Γ used by Robertson in his arXiv publication [7] taken from Ref. [13], although there seems to be in some cases better values in the literature [14–18]. The last two columns give the relative probabilities of the one- and the two-hole states in relation to $3s_{1/2}$ in percent for ^{163}Dy of the present work (P-Fae) and the publication of Robertson (P-Rob) [7]. One finds surprisingly large differences for the two-hole probabilities from those of Robertson [7]. To ensure that the present values are correct, three two-hole probabilities with about the largest differences from those of Robertson have also been calculated by hand. The two-hole probabilities are extremely sensitive to the overlap between the relativistic electron orbitals in Ho and Dy with the same quantum numbers $|n,\ell,j\rangle$. In a very rough approximation, Eq. (1) provides a lever to enlarge a small change in the overlap into a large change in the two-hole probability. The difference between the Robertson results and the present approach is largest for the outermost electron orbitals for the second hole. One expects for the slightly bound states $5s_{1/2}$, $5p_{1/2}$, and $5p_{3/2}$ the overlaps in Xe and Ho to have the largest differences, because these states are much weaker bound in Xe than in Ho. See Table III.

One-hole	Two-hole	E_c (eV)	Γ (eV)	P-Fae (%)	P-Rob (%)
$3s_{1/2}$	–	2041.8	13.2	100	100
$3s_{1/2}$	$4s_{1/2}$	2474.2	13.2	0.167	0.075
$3s_{1/2}$	$4p_{1/2}$	2385.3	13.2	0.103	0.11
$3s_{1/2}$	$4p_{3/2}$	2350.0	13.2	0.163	0.25
$3s_{1/2}$	$4d_{3/2}$	2201.8	13.2	0.930	1.05
$3s_{1/2}$	$4d_{5/2}$	2201.8	13.2	0.126	1.62
$3s_{1/2}$	$4f_{5/2}$	2050.4	13.2	0.165	0.0
$3s_{1/2}$	$4f_{7/2}$	2047.0	13.2	0.182	0.0
$3s_{1/2}$	$5s_{1/2}$	2091.1	13.2	0.132	1.36
$3s_{1/2}$	$5p_{1/2}$	2072.6	13.2	0.128	3.12
$3s_{1/2}$	$5p_{3/2}$	2065.9	13.2	0.185	7.31
$3p_{1/2}$	–	1836.8	6	5.080	5.26
$3p_{1/2}$	$4s_{1/2}$	2269.2	6	0.005	0.004
$3p_{1/2}$	$4p_{1/2}$	2180.3	6	0.009	0.006
$3p_{1/2}$	$4p_{3/2}$	2145.0	6	0.007	0.014
$3p_{1/2}$	$4d_{3/2}$	1996.8	6	0.005	0.057
$3p_{1/2}$	$4d_{5/2}$	1996.8	6	0.005	0.087
$3p_{1/2}$	$4f_{5/2}$	1845.4	6	0.005	0.00
$3p_{1/2}$	$4f_{7/2}$	1842.0	6	0.012	0.00
$3p_{1/2}$	$5s_{1/2}$	1886.1	6	0.005	0.072
$3p_{1/2}$	$5p_{1/2}$	1887.6	6	0.008	0.165
$3p_{1/2}$	$5p_{3/2}$	1860.9	6	0.008	0.386

TABLE II. Continuation of Table I with one- and two-hole states in ^{163}Dy.

One-hole	Two-hole	E_c (eV)	Γ (eV)	P-Fae (%)	P-Rob (%)
$4s_{1/2}$	–	409.0	5.4	24.40	23.29
$4s_{1/2}$	$4s_{1/2}$	841.4	5.4	0.021	0.001
$4s_{1/2}$	$4p_{1/2}$	752.5	5.4	0.052	0.004
$4s_{1/2}$	$4p_{3/2}$	717.2	5.4	0.091	0.01
$4s_{1/2}$	$4d_{3/2}$	569.0	5.4	0.088	0.077
$4s_{1/2}$	$4d_{5/2}$	569.0	5.4	0.125	0.123
$4s_{1/2}$	$4f_{5/2}$	417.6	5.4	0.027	0.0
$4s_{1/2}$	$4f7/2$	414.2	5.4	0.023	0.0
$4s_{1/2}$	$5s_{1/2}$	458.3	5.4	0.066	0.254
$4s_{1/2}$	$5p_{1/2}$	439.8	5.4	0.039	0.629
$4s_{1/2}$	$5p_{3/2}$	433.1	5.4	0.058	1.502
$4p_{1/2}$	–	328.3	5.3	1.220	1.19
$4p_{1/2}$	$4p_{1/2}$	671.8	5.3	0.001	0.0001
$4p_{1/2}$	$4p_{3/2}$	636.5	5.3	0.004	0.0005
$4p_{1/2}$	$4d_{3/2}$	488.3	5.3	0.005	0.004
$4p_{1/2}$	$4d_{5/2}$	488.3	5.3	0.006	0.006
$4p_{1/2}$	$4f_{5/2}$	336.9	5.3	0.002	0.0
$4p_{1/2}$	$4f_{7/2}$	328.3	5.3	0.001	0.0
$4p_{1/2}$	$5s_{1/2}$	377.6	5.3	0.002	0.013
$4p_{1/2}$	$5p_{1/2}$	359.1	5.3	0.004	0.031
$4p_{1/2}$	$5p_{3/2}$	352.4	5.3	0.002	0.076
$5s_{1/2}$	$5s_{1/2}$	44.7	3	3.200	3.45
$5p_{1/2}$	$5p_{1/2}$	21.1	3	0.157	0.15

TABLE III. Ionization energies and two-hole probabilities $P(\%)$ (6) relative to the $3s_{1/2}$ state comparing Xe with Ho. A small reduction of the overlap, which is typically for well-bound electron orbitals $\langle Z, n, \ell, j \mid Z-1, n, \ell, j\rangle = 0.999$, by an assumed value of 2% produces by the lever of Eq. (1) a large increase of the two-hole probability. The reduction of the overlap for going from an atom with Z to an atom with $Z-1$ is largest for very lightly bound electrons. The $5s_{1/2}$, $5p_{1/2}$, and $5p_{3/2}$ states are in xenon with $Z = 54$ only with half the energy E bound as in holmium with $Z = 67$. The binding energies of the holmium orbitals in parenthesis are taken from Robertson [7]. The other values are from the literature [13,15–18]. A decrease of the overlaps in xenon by an assumed 2% to 0.979 relative to holmium increases the probability for the second hole P(2-hole) by a factor of 20. This factor increases the two-hole probabilities in these states to roughly the values of Robertson [7] (see Tables I and II), who used the results of Carlson and Nestor [9] calculated for xenon. It should be stressed that the two-hole probabilities in this work are not calculated by the very rough Eq. (1) but by the more accurate expression (21).

	E (eV) xenon	E (eV) holmium
$5s_{1/2}$	23.3	49.9
$5p_{1/2}$	13.4	26.3(30.8)
$5p_{3/2}$	12.1	26.3(24.1)
Overlap	for (−2%) 0.979; P(2-hole)	for 0.999; P(2-hole)
$j = 1/2$	8.1%	0.4%
$j = 3/2$	15.6%	0.8%

overlaps from xenon to holmium-dysprosium needs to be only 1% to yield a difference of a factor of 10 or more for the two-hole probabilities. For one hole in the dysprosium state $3s1/2$ or $4s1/2$ we have the following:

$$\text{hole in } 3s_{1/2}\text{: } \langle \text{Ho},3s_{1/2}|\text{Dy},3s_{1/2}\rangle = 0.999\,390,$$
$$\langle \text{Ho},4s_{1/2}|\text{Dy},4s_{1/2}\rangle = 0.999\,332; \quad (2)$$
$$\text{hole in } 4s_{1/2}\text{: } \langle \text{Ho},3s_{1/2}|\text{Dy},3s_{1/2}\rangle = 0.999\,377,$$
$$\langle \text{Ho},4s_{1/2}|\text{Dy},4s_{1/2}\rangle = 0.998\,870. \quad (3)$$

(All numbers in this work are calculated in double precision.)

(v) For the probabilities of the one-hole states $3s_{1/2}$ ($M1$), $3p_{1/2}$ ($M2$), $4s_{1/2}$ ($N1$), $4p_{1/2}$ ($N2$), $5s_{1/2}$ ($O1$), $5p_{1/2}$ ($O2$), and $6s_{1/2}$ ($P1$), which determine the main structure of the spectrum, the overlap and exchange corrections are included according to Faessler *et al.* [4].

(vi) In solving the DHF electron wave functions [2,10–12] the nuclear charge distribution is included in the Fermi parametrization determined by electron-nucleus scattering.

(vii) The nuclear matrix element for electron capture integrates the charge of the captured Ho electron over the nucleus with the weight $\psi^2(r)_{e,n,\ell,j}r^2$. Thus, for the capture probability the value $\psi^2(R)_{e,n,\ell,j}R^2$ is taken (R is the nuclear radius) and not the value $\psi^2(r = 0.0)_{e,n,\ell,j}$ at $r = 0.0$, which has the r^2 weight zero.

(viii) The formulas are derived in second quantization including automatically the full antisymmetrization. This formulation allows one not only to describe two-hole states but also to extend the description for three-hole and even more hole states.

II. DESCRIPTION OF ELECTRON CAPTURE AND THE ATOMIC WAVE FUNCTIONS

The bolometer spectrum of the deexcitation of ^{163}Dy after electron capture in ^{163}Ho can be expressed as in Refs. [3] and [4] assuming Lorentzian line profiles:

$$\frac{d\Gamma}{dE_c} \propto \sum_{i=1,\ldots,N_\nu} (Q - E_c)U^2_{e,i}\sqrt{(Q-E_c)^2 - m^2_{\nu,i}} \times \sum_{f=f'} \lambda_0 B_f \frac{\Gamma_{f'}}{2\pi}\frac{1}{(E_c - E_{f'})^2 + \Gamma^2_{f'}/4}. \quad (4)$$

Here $Q = 2.3$ to 2.8 keV [5,14,19–21], with a recommended value [22] $Q = (2.55 \pm 0.016)$ keV; $U^2_{e,i}$ is the probability for the admixture of different neutrino mass eigenstates $i = 1,\ldots,N_\nu$ into electron neutrinos; E_c is the excitation energy of the final dysprosium; B_f are the overlap and exchange corrections; λ_0 contains the nuclear matrix element squared [23]; $E_{f'}$ are the one- and two-hole excitation energies in dysprosium; and $\Gamma_{f'}$ are the widths of the one- and two-hole states in dysprosium [4].

Here, as in all other calculations for the deexcitation of Dy after electron capture, a Lorentzian shape is assumed. This is probably a good description. Holmium in the ECHo

experiment is built into a gold film positioned as an interstitial or it occupies a position in the gold lattice. A Gaussian shape would be expected in a gas from Doppler broadening. Even collision and pressure broadening yield usually a Lorentzian profile. But because the shape of the resonance lines are important for the determination of the neutrino mass, the line shapes should be studied in the future more carefully.

Results of the ECHo Collaboration [14] for electron capture in ^{163}Ho to ^{163}Dy yield the following Q value:

$$Q(\text{ECHo}) = (2.80 \pm 0.08)\,\text{keV}. \tag{5}$$

The highest two-hole state in Dy has an energy of 2.474 keV (see Table I), far below the Q value. So three-hole and multihole states (and perhaps also states from configuration mixing), which can be higher in energy, might be more dangerous for the determination of the neutrino mass.

We assume, that the total atomic wave function can be described by a single Slater determinant. B_f takes into account the overlap and the exchange terms between the parent $|G\rangle$ and the daughter atom in the state $|A'_f\rangle$ with a hole in the electron state $|f'\rangle$. We use the sudden approximation like Faessler *et al.* [24]. B_f is the overlap and exchange correction for the electron capture probability from the state f relative to the capture from $3s_{1/2}$ in Ho with one hole in f' in the Dy atom, given in Eq. (6) in the Vatai approximation [25,26]. But the numerical values used here are calculated with the full overlap and exchange corrections of Faessler *et al.* [4]:

$$B_f = \frac{|\psi_f(R)\langle A'_f|a_f|G\rangle|^2}{|\psi_{3s1/2}(R)|^2} = P_f \frac{|\psi_f(R)|^2}{|\psi_{3s1/2}(R)|^2}. \tag{6}$$

For two-hole final states one has to multiply Eq. (6) according to Eq. (15) with the probability to form a second hole characterized by the quantum numbers "p'". One has to replace $\langle A'_{f'}|a_i|G\rangle$ by

$\langle A'_{f',p';q'}|a_i|G\rangle$ with the two electron holes f' and p' and the additional electron particle q' in dysprosium above the Fermi surface F. The probability for the leading expression (Wick [27] contracted) to form one hole in Dy in $f' = f = i$ is

$$P_f = |\langle A'_{f'}|a_{i=f}|G\rangle|^2 \approx \prod_{k=1,\ldots,Z;\neq f} |\langle k'|k\rangle|^2. \tag{7}$$

The corresponding probability for two final hole states f' and p' and an additional electron in q' summed over all $q' > F$ of the unoccupied bound and the continuum states is

$$P_{p'/f'} = \sum_{q'>F} |\langle A'_{f',p';q'}|a_i|G\rangle|^2. \tag{8}$$

The antisymmetrized Slater determinants for the wave functions of the initial holmium in the ground state $|G\rangle$ and the excited one-electron-hole state $|A'_f\rangle$ in dysprosium read in second quantization as follows:

$$|G\rangle = a_1^\dagger a_2^\dagger a_3^\dagger \cdots a_Z^\dagger |0\rangle, \tag{9}$$

$$|A'_f\rangle = a_1'^\dagger a_2'^\dagger \cdots a_{f'-1}'^\dagger a_{f'+1}'^\dagger \cdots a_Z'^\dagger |0\rangle. \tag{10}$$

The antisymmetrized two-hole state in Dy is

$$|A'_{p',f'}\rangle = a_1'^\dagger a_2'^\dagger \cdots a_{f'-1}'^\dagger a_{f'+1}'^\dagger \cdots a_{p'-1}'^\dagger a_{p'+1}'^\dagger \cdots a_Z'^\dagger a_{q'>F}'^\dagger |0\rangle. \tag{11}$$

The primes with the dagger indicate the single-electron spinor creation operators for the daughter nucleus (dysprosium) with one electron hole in the single-particle state $|f'\rangle$ in Eq. (10) and two holes $|f'\rangle$ and $|p'\rangle$ in Eq. (11). The following expressions have to be calculated with the help of Wick's theorem [27]:

$$P_f = |\langle A'_f|a_i|G\rangle|^2 = |\langle 0|a'_Z a'_{Z-1}\cdots a'_{f+1}a'_{f-1}\cdots a'_1 \cdot a_f \cdot a_1^\dagger a_2^\dagger a_3^\dagger \cdots a_Z^\dagger|0\rangle|^2, \tag{12}$$

$$P_{p/f} = |\langle A'_{p',f'}|a_f|G\rangle|^2 = \sum_{q'>F} |\langle 0|a'_{q'}a'_Z\cdots a'_{p'+1}a'_{p'-1} \cdots a'_{f+1}a'_{f-1}\cdots a'_1 \cdot a_f \cdot a_1^\dagger a_2^\dagger a_3^\dagger \cdots a_Z^\dagger|0\rangle|^2. \tag{13}$$

One considers the Wick contractions as an expansion with the "nondiagonal" overlaps as small parameters. The leading term is the expression without nondiagonal overlaps. The leading expression (without the sub-leading exchange terms, which contain at least one nondiagonal overlap in the amplitude) is obtained in Eq. (12) for electron capture in holmium from the state i if the captured electron i in Ho has the same quantum numbers n, ℓ, and j as the final hole state f' in Dy, i.e., for the quantum numbers $i = f = f'$. The probability for two-hole states, Eq. (13), is next to the leading order, because it contains always at least one nondiagonal overlap $\langle q'|p\rangle$ for the amplitude and the square for the probability. If the sequence of f' and p' is reversed in dysprosium the Fermion creation operators produce automatically a "$-$" sign for the amplitude, which does not matter for the probability.

III. DERIVATION OF THE PROBABILITIES

It has been already stressed that the leading contribution for the one-hole state in Eq. (12) and for the two-hole state in Eq. (13) is obtained if the orbital quantum numbers for the captured electron in holmium, $|i\rangle = |n,\ell,j,m\rangle$, are the same as the hole quantum numbers in Dy, $|f'\rangle = |n',\ell',j',m'\rangle$; thus $i = f' = f$ and $n = n'$, $\ell = \ell'$, $j = j'$, and $m = m'$.

The leading expression for the probability to excite the hole state in Dy corresponding to the quantum numbers of the state of the captured electron in holmium is

$$P_f = |\langle A'_f|a_f|G\rangle|^2 = \prod_{k=k'<F,\neq f} \langle k'|k\rangle|^2 = \prod_{(n,\ell,j)(\text{Ho=Dy})<F_{\text{Dy}}} |\langle (nlj)_{\text{Dy}}|(n,\ell,j)_{\text{Ho}}\rangle|^{2N_{n,\ell,j}} \tag{14}$$

The definition of $N_{n,\ell,j}$ is given in Eq. (23). $(n,\ell,j)_{\text{Ho}}$ and $(n,\ell,j)_{\text{Dy}}$ indicate electrons in the Ho atom and in the Dy atom with the same quantum numbers. Such states have a large overlap only slightly below unity.

For the following one needs some elementary laws of probability calculus:

$$P(A \text{ and } B) = P(A)\cdot P(B),$$
$$P(A \text{ or } B) = P(A) + P(B), \quad \text{if } A \text{ and} B \text{ exclude each other.} \tag{15}$$

If one wants to include the leading contribution for two holes in the final Dy atom, one must multiply expression P_f

in Eq. (14) with the probability $P_{p/f}$ to form an additional electron particle $q' > F$ (F is the Fermi surface) and an electron hole state $p' < F$. The excited electron q' can be in an unoccupied bound state or in the continuum of the Dy atom:

$$\begin{aligned} P_{p/f}(q' > F) &= |\langle 0|a'_{q'}a'_Z \cdots a'_{p'+1}a'_{p'-1} \cdots a'_{f'+1}a'_{f'-1} \\ &\quad \cdots a'_1 a_f a_1^+ \cdots a_Z^+|0\rangle|^2 \\ &= |\langle A'_{p',f'<F;q'>F}(2\text{ holes})|a_f|G\rangle|^2 \\ &\approx |\langle q'_{>F}|p_{<F}\rangle \prod_{k=1\ldots Z\neq f,p} \langle k'|k\rangle|^2, \end{aligned} \tag{16}$$

where q' is an empty electron orbit in Dy, into which the electron p is scattered, and p is the occupied state in Ho, from which this electron is removed. Here again k and k' and also f and f' and p and p' stand for the same electron quantum numbers n, ℓ, and j in the parent atom k, f, and p and the daughter atom k', f', and p'. The product over k runs over occupied states $k' = k = (n_k, \ell_k, j_k, m_k)$ in Ho and Dy with the exemption of $f = (n_f, \ell_f, j_f, m_f)$. q', an empty state in Dy, can be bound or in the continuum. If q' is in the continuum, one speaks of "shake off." Because now a nondiagonal overlap is involved in Eq. (16) with $\langle q'_{\rm Dy}|p_{\rm Ho}\rangle$ already in the amplitude and this expression must be squared for the probability, the two-hole contributions are reduced by a nondiagonal overlap squared. If one exchanges the states f' and p', one obtains an additional "$-$" sign. But because one has to square the expression, a phase is irrelevant.

To evaluate the probability for an additional electron particle-hole state (16) one sums incoherently over all unoccupied states q' (this assumes that the different two-hole excitations do not influence each other):

$$\begin{aligned} P_{f',p'} &= \sum_{q'>F} |\langle p_{<F,\rm Ho}|q'_{>F,\rm Dy}\rangle\langle q'_{>F,\rm Dy}|p_{<F,\rm Ho}\rangle| \\ &\quad \times \prod_{k=k'<F_{\rm Dy}\neq f,p} |\langle k'_{\rm Dy}|k_{\rm Ho}\rangle|^2 \end{aligned} \tag{17}$$

Here, as stressed above, the sum over q' runs only over the unoccupied bound and continuum states in Dy. One can now use the completeness relation to shift the sum over q' to states away from the continuum states, which one can more easily calculate. One divides the completeness relation into two pieces, up to the last occupied state below the Fermi surface F and all states above the last occupied state including also the continuum:

$$1 = \sum_{q'<F} \langle p|q'\rangle\langle q'|p\rangle + \sum_{q'>F} \langle p|q'\rangle\langle q'|p\rangle. \tag{18}$$

The sum in Eq. (17) is the last part of Eq. (18) and one can transcribe Eq. (17) into

$$\begin{aligned} P_{p/f} &= \left(1 - \sum_{q'<F} \langle p_{\rm Ho}|q'_{\rm Dy}\rangle\langle q'_{\rm Dy}|p_{\rm Ho}\rangle\right) \\ &\quad \times \prod_{k=k'<F_{\rm Dy};\neq p,f} \langle k'_{\rm Dy}|k_{\rm Ho}\rangle. \end{aligned} \tag{19}$$

In the literature one uses often the Vatai approximation [25,26]: Exchange corrections have already been neglected in the previous expressions. In addition one assumes that the overlaps of electron wave functions in the parent atom and the daughter atom with the same quantum numbers [given in the product term in Eq. (19)] can be approximated by unity. Typically the overlaps have values [4] $\langle k'_{\rm Dy}|k_{\rm Ho}\rangle \approx 0.999$ and thus for Dy minus two holes $0.999^{64} \approx 0.94$. In the Vatai approximation [26] one replaces this value by 1.0:

$$\begin{aligned} P_{p/f} &= \left(1 - \sum_{q'<F} \langle p_{\rm Ho}|q'_{\rm Dy}\rangle\langle q'_{\rm Dy}|p_{\rm Ho}\rangle\right) \\ &= \Bigg(1 - \langle p_{\rm Ho}|p'_{\rm Dy}\rangle\langle p'_{\rm Dy}|p_{\rm Ho}\rangle \\ &\quad - \sum_{q'<F,\neq p'} \langle p_{\rm Ho}|q'_{\rm Dy}\rangle\langle q'_{\rm Dy}|p_{\rm Ho}\rangle\Bigg). \end{aligned} \tag{20}$$

The physics of the two terms subtracted from 1 in Eq. (20) is as follows: The first subtracted term gives the probability that the state p' in Dy is occupied. The second terms take into account the Pauli principle and prevent the electrons from being moved into occupied states in Dy. The single electron states like $|p\rangle = |n,\ell,j,m\rangle$ include also the angular projection quantum number m. This projection is irrelevant for the description of the data. The first subtracted term in Eq. (20) gives the probability that a specific magnetic substate m' is occupied in p'. The probability that all magnetic substates of p' are occupied is an "and" situation (15). The probabilities for the substates have to be multiplied and one obtains the Nth power of the single-electron probability with $N_{p'} = N_{n,\ell,j;p'} = (2j+1)_{p'}$, $|\langle (n,\ell,j)_{p,\rm Ho}|(n,\ell,j)_{p',\rm Dy}\rangle|^{2N_{n,\ell,j;p'}}$:

$$\begin{aligned} P_{p/f} &= (1 - |\langle (n,\ell,j)_{p,\rm Ho}|(n,\ell,j)_{p',\rm Dy}\rangle|^{2\cdot N_{p'}} \\ &\quad - \sum_{(n,\ell,j)_{q',\rm Dy};\neq p'<F} \frac{N_{n,\ell,j}N_{n',\ell,j}}{2j+1} \\ &\quad \times |\langle (n,\ell,j)_{p,\rm Ho}|(n,\ell,j)_{q',\rm Dy}\rangle|^2) \end{aligned} \tag{21}$$

for n and n' with

$$N_{n,\ell,j} = 2j+1. \tag{22}$$

However, for the primary hole state f and the $4f_{7/2}$ state one has special factors:

$$N_{(n,\ell,j)_f} = 2j_f \text{ and } N_{4f_{7/2}} = 5. \tag{23}$$

Here $|f\rangle$ is the orbital in Ho from which the electron is originally captured. The electron p' is moved to $4f_{7/2}$ with now five electrons in this orbit to guarantee the correct number of electrons. $N_{n,\ell,j}/(2j+1)$ is the averaged probability to find an electron in the $|p,n,\ell,j,m\rangle$ orbital and $N_{n',\ell,j}$ is the number of electrons in the $|q',n',\ell,j\rangle$ state. For the probability of the second hole we used the Vatai [25,26] approximation with the overlaps of corresponding electron wave functions with the same quantum numbers in Ho and Dy equal to unity and we neglected the exchange corrections. For the diagonal overlaps of the order of ≈ 0.999 this is a good approximation.

Here some details of the determination of the one- and two-hole probabilities are listed:

(i) In the formation of the first-hole state in orbital f in Ho and f' in Dy, the electron can be captured from each projection quantum number m. One has an "or" situation. According to Eq. (15) the probabilities add up. However, because one has capture only from the $s_{1/2}$ and $p_{1/2}$ states, this yields a common factor of 2 in the amplitude and thus is not relevant for the relative probabilities.

(ii) The probability amplitude for the second hole is calculated in the sudden approximation [24] by the overlap of the ground state of Ho with the captured electron f removed with Dy with a hole in f' and the particle-hole excitation $(q'^1 p'^{-1})$. The overlap squared $|\langle (n,\ell,j)_{p,\mathrm{Ho}} | (n,\ell,j)_{p',\mathrm{Dy}} \rangle|^2$ gives the probability, that a specific magnetic substate $m_{p'}$ is occupied. To obtain the probability that all magnetic substates of p' are occupied, one has the "and" situation (15), which requires one to multiply all these probabilities with each other, which yields the power of $N_{(n,\ell,j)p'}$.

(iii) The second subtracted term in Eq. (21) takes care of the Pauli principle of the occupied states excluding p'. One has an "or" situation. Thus one obtains a factor of $N_{n,\ell,j}$ according to Eqs. (15) and (23).

(iv) The one hole f' and the particle-hole excitation $(q'^1 p'^{-1})$ are in an "and" situation. Thus the probabilities have to be multiplied $P(f'^{-1})P(q'^1, p'^{-1})$ according to Eq. (15). One multiplies the probabilities (14) with Eq. (16). These probabilities relative to $3s_{1/2}$ (6) are listed in Tables I and II.

IV. COMPARISON WITH CARLSON AND NESTOR

Carlson *et al.* [8] and Carlson and Nestor [9] derived by physics arguments for the antisymmetrization and the Pauli principle the probability to excite apart from a hole in f' also an additional particle-hole state:

$$P_{\mathrm{Carlson};f,p} = (1 - (|\langle (n,\ell,j)_{p',\mathrm{Dy}} | (n,\ell,j)_{p,\mathrm{Ho}} \rangle|^2)^{N_{n\ell j}} - \sum_{n'<F;\neq n'_p} \frac{N_{n,\ell,j} N_{n',\ell,j}}{2j+1} \times |\langle n',\ell,j(\mathrm{Dy}) | n,\ell,j(\mathrm{Ho}) \rangle|^2). \quad (24)$$

The definition of $N_{n,\ell,j}$ is given in Eq. (23). $(n,\ell,j)_{p,\mathrm{Ho}}$ and $(n,\ell,j)_{p',\mathrm{Dy}}$ indicate electrons in the Ho atoms and in the Dy atoms with the same quantum numbers.

Equations (21) and (24) are in the Vatai approximation [25,26] identical with the expressions of Carlson and Nestor [9]. That means one neglects exchange terms and assumes that the overlaps of equivalent electron orbitals with the same quantum numbers in the parent atom and in the daughter atom are equal to unity. Thus we have in the Vatai approximation [25,26] verified the formula of Carlson and Nestor [9] including here more rigorously the antisymmetrization and the Pauli principle and showing also expressions beyond the Vatai approximation.

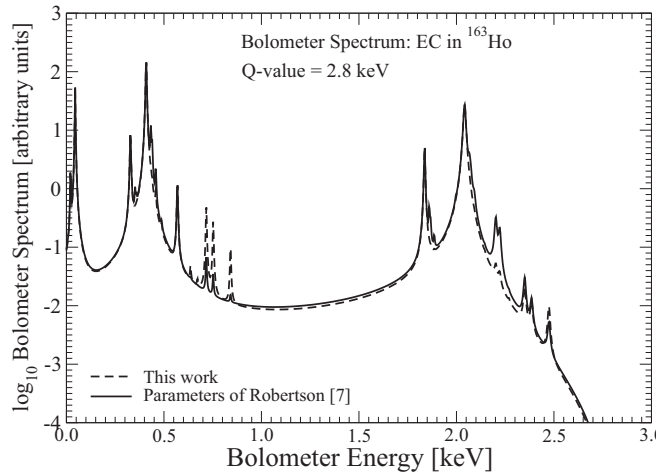

FIG. 1. Logarithmic$_{10}$ (with basis 10) bolometer spectra (4) and (21) for the one- and two-hole probabilities calculated in this work (dashed line) and with the parameters of Robertson (solid line) [7] with the assumed Q value = 2.8 keV for the bolometer energy between 0.0 and 2.8 keV. Apart from the excitation of one-hole states in ^{163}Dy after electron capture in ^{163}Ho, the excitations of the two-hole states in ^{163}Dy are also included. The logarithmic$_{10}$ plot stresses the effect of the two-hole states. In a linear plot (see Fig. 2) the two-hole states are hardly to be seen. The values at the ordinate have to be read as 10^{ordinate}. So "-2" is 10^{-2}.

The logarithmic (with basis 10) bolometer spectra (4) and (21) for the one- and two-hole probabilities of Fig. 1 is calculated with the parameters of Robertson [7] and a Q value = 2.8 keV for the energy between 0.0 and 2.8 keV. In Fig. 2 the one-hole energies and the widths from Table IV are used. The excitations of one-hole states in ^{163}Dy after electron capture in ^{163}Ho and also the excitations of two-hole states in Dy are included. For the widths of the resonances we assumed in this work, if they are not known experimentally, the estimates of Robertson [7] to allow a better comparison. In a linear plot of the bolometer spectrum the two-hole excitations are hard to see and the spectrum calculated in this work and the one calculated with the probabilities of Robertson [7] and Carlson and Nestor [9] look almost identical, although the two-hole probabilities are in some cases very different as shown in Tables I and II. The two-hole modifications of the bolometer spectrum show up clearly in a logarithmic plot, but are suppressed in a figure with a linear ordinate.

In Fig. 2 the theoretical results for the bolometer spectrum in electron capture in ^{163}Ho to ^{163}Dy of this work are compared with the experimental data of Ranitzsch *et al.* [28] and Gastaldo *et al.* [29] in a linear plot assuming a Q value of 2.8 keV.

In Fig. 3 the upper end (2.70 to 2.80 keV) of the theoretical linear bolometer spectrum of the present approach including one- and two-hole states is shown for an electron neutrino mass of 0.0 and 2 eV. A similar result is obtained for the following Q values: $Q = 2.3$ keV and $Q = 2.5$ keV.

What happens if the Q value falls within the width of a two-hole resonance? This situation is displayed in Fig. 4. The two-hole resonance $3s_{1/2}, 4p_{3/2}$ lies at 2.350 keV with a width of $\Gamma = 13.2$ eV. The figure shows the upper part of the bolometer

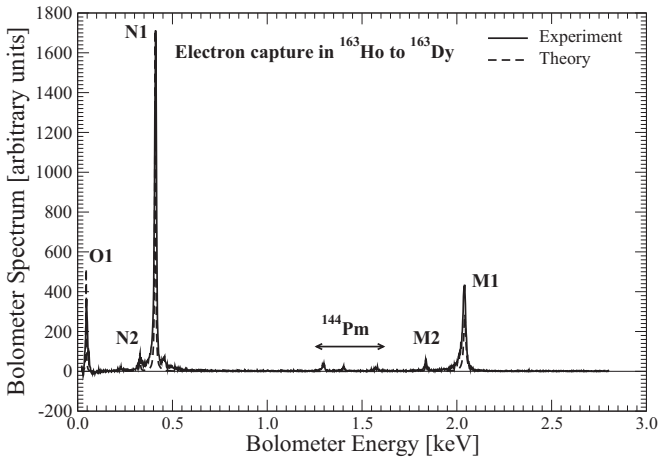

FIG. 2. Experimental (solid line) and theoretical (dashed line) linear bolometer spectra (4) and (21) for electron capture in ^{163}Ho to ^{163}Dy with the Q value = 2.8 keV [see Eq. (5)] including the one- and two-hole probabilities calculated in this work and compared to the Heidelberg experiment of Ranitzsch *et al.* [28] and Gastaldo *et al.* [29] for the total bolometer energy from 0.02 to 2.80 keV. The theoretical spectrum is normalized to the data of the $N1$ ($4s_{1/2}$) peak at 0.42 keV. The three small experimental lines between 1.2 and 1.6 keV originate from small admixtures of ^{144}Pm. The experimental counts are binned in 2-eV intervals. Due to background subtraction the number of counts in some bins can be negative. In some regions of the energy the number of counts per bin is zero or one. Due to negative and zero counts in a bin it is not possible to plot the data logarithmically as in Fig. 1, which would show the small effects of the two-hole excitations in Dy better. The theoretical spectrum is calculated for zero neutrino mass and with the excitation and the width of the one-hole states of the ECHo Collaboration [28,29] listed in Table IV.

spectrum from 2.345 to 2.355 keV for a neutrino mass of $m_\nu = 0$ eV and $m_\nu = 2$ eV.

Figure 5 shows the upper end of a theoretical spectrum with a mixture of two mass eigenstates for the electron neutrino. The mixing probabilities are adopted from Capozzi *et al.* [30]. The onset of the 10-eV admixture at 2.790 keV can be seen.

The importance of excited states in Dy for the neutrino mass determination does not depend on whether they are one-hole, two-hole, or multihole states or whether they are of a different nature. Under the assumption that the shape of the resonances are Lorentzian, the importance of a specific state for the determination of the neutrino mass can be seen

TABLE IV. The electron binding energies and widths of hole states in ^{163}Ho from the literature [13,15–18] and recent ECHo data [28,29]. Electrons below $3s_{1/2}$ cannot be captured in ^{163}Ho. Due to the Q value of about 2.8 keV they are energetically forbidden.

	n,ℓ,j	$E_{\rm lit}$ (keV)	$E_{\rm ECHo}$ (keV)	$\Gamma_{\rm lit}$ (eV)	$\Gamma_{\rm ECHo}$ (eV)
$M1$	$3s_{1/2}$	2.047	2.040	13.2	13.7
$M2$	$3p_{1/2}$	1.836	1.836	6.0	7.2
$N1$	$4s_{1/2}$	0.420	0.411	5.4	5.3
$N2$	$4p_{1/2}$	0.340	0.333	5.3	8.0
$O1$	$5s_{1/2}$	0.050	0.048	5.0	4.3

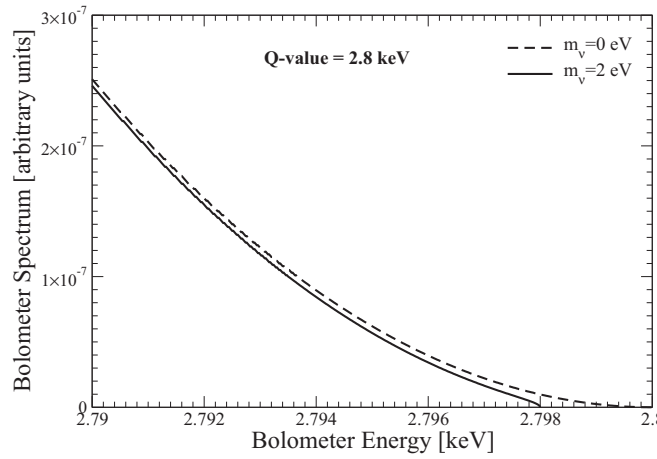

FIG. 3. The upper 10 eV of the bolometer spectrum from 2.790 to the Q value = 2.800 keV for neutrino masses $m_\nu = 0.0$ eV (dashed line) and $m_\nu = 2$ eV (solid line).

from Eq. (4). A measure of the importance of a state for the determination of the neutrino mass is

$$\text{importance} \propto \frac{B_f \Gamma_{f'}}{(Q - E_{f'})^2 + \Gamma_{f'}^2/4} \approx \frac{B_f \Gamma_{f'}}{(Q - E_{f'})^2}. \quad (25)$$

The dependence on the resonance energy $E_{f'}$ is $(Q - E_{f'})^{-2}$, if the distance of the energy to the Q value is larger than the width. So states near the Q value normally have the largest influence on the determination of the neutrino mass. In general one needs a simultaneous fit of the neutrino mass, the Q value, and the parameters ($E_{f'}$, $B_{f'}$, and the width $\Gamma_{f'}$) of the most important resonance (or even resonances). This

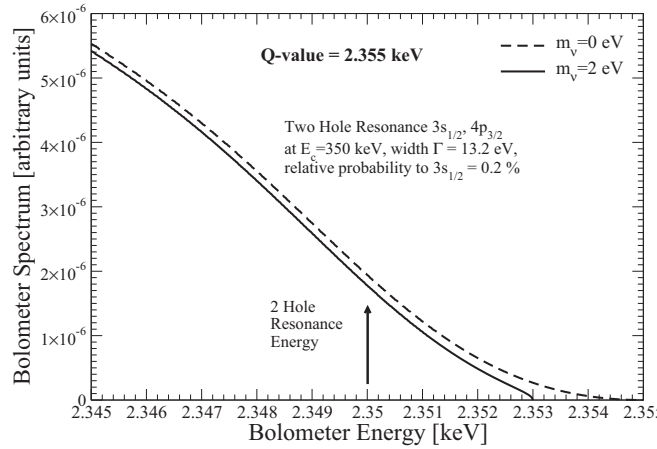

FIG. 4. The upper 10 eV of the bolometer spectrum from 2.345 keV to the assumed Q value = 2.355 keV for neutrino masses $m_\nu = 0.0$ eV (dashed line) and $m_\nu = 2$ eV (solid line). The two-hole state $3s_{1/2}, 4p_{3/2}$ at $E_c = 2.350$ keV in ^{163}Dy is just below the assumed Q value = 2.355 keV within the width $\Gamma = 13.2$ eV. In a simultaneous fit of the neutrino mass and the Q value, also the position, the width, and the strength of the resonance state must also be included. A finite neutrino mass produces at the upper end of the spectrum a special fingerprint, which cannot be produced by a resonance state. Thus one can hope, that even in this situation the upper end of the spectrum shows the fingerprint of a finite neutrino mass.

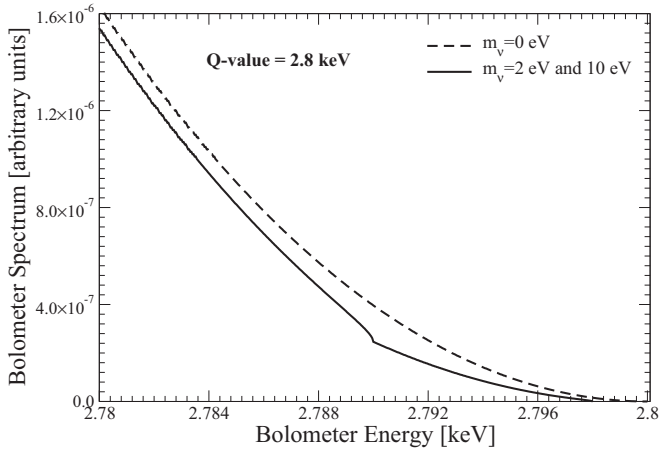

FIG. 5. The upper 20 eV of the bolometer spectrum in ^{163}Dy for a neutrino with mass $m_\nu = 0$ eV (dashed line) and an electron neutrino, which is a mixture of two mass eigenstates with $m_\nu = 2$ eV and $m_\nu = 10$ eV (solid line) for the assumed Q value = 2.8 keV. The mixing coefficients are adopted from Ref. [30] assuming only mixing of two neutrinos with probabilities of $U^2_{e,1}(2\text{ eV}) = 0.636$ and $U^2_{e,2}(10\text{ eV}) = 0.364$. The neutrino with $m_\nu = 0$ eV is assumed to have $U^2_{e,1} = 1.0$ and $U^2_{e,2} = 0.0$. The onset of the heavy neutrino of $m_\nu = 10$ eV at $(Q - 10)$ eV = 2.790 keV can be seen in the theoretical spectrum. Finite experimental energy resolution will at least partially smear out this effect.

makes the determination of the neutrino mass very difficult or perhaps even impossible.

To analyze how many and which parameters must be fitted to the upper end of the experimental spectrum, we introduce the definitions ΔE_C and $\Delta E_{f'}$ in Eq. (26), and we assume that only one resonance determines the upper end of the spectrum near the Q value and that the profile of this line is Lorentzian:

$$E_C = Q - \Delta E_C, \quad E_{f'} = Q - \Delta E_{f'}. \tag{26}$$

ΔE_C describes the variable energy and $\Delta E_{f'}$ the distance of the leading resonance to the Q value, and $\Gamma_{f'}$ is the width of this resonance:

$$\frac{d\Gamma}{dE_c} \propto (Q - E_c)\sqrt{(Q - E_c)^2 - m_\nu^2}\,\frac{S}{(E_c - E_{f'})^2 + \Gamma^2_{f'}/4}$$
$$= \Delta E_C\sqrt{\Delta E_C^2 - m_\nu^2}\,\frac{S}{(\Delta_{f'} - \Delta E_C)^2 + \Gamma^2_{f'}/4}. \tag{27}$$

Here $S \propto \lambda_0 B_f \Gamma_{f'}$ is the strength of the resonance.

An estimate shows that the one-hole states play the decisive role in the behavior at the Q value, assuming that the more accurate value of $Q = 2.8$ keV of the ECHo Collaboration [14] is correct. The relative weight 174 for the highest one-hole state $3s_{1/2}$ at 2.0418 keV with $P_{\text{1-hole}} = 100\%$ is at the Q value, the important area for the neutrino mass, by a factor of 100 larger than the weight 1.6 of the highest two-hole state at 2.4742 keV with $P_{\text{2-hole}} = 0.167$ % from Table I:

$$\text{relative weight} \propto \frac{P_{\text{1-hole}}\%}{(Q - E_{f'})^2} = \frac{100\%}{(2.80 - 2.04)^2} = 174,$$

$$\text{relative weight} \propto \frac{P_{\text{2-hole}}\%}{(Q - E_{f'})^2} = \frac{0.167\%}{(2.80 - 2.47)^2} = 1.6. \tag{28}$$

The widths of the one- and the two-hole states of the highest energies are assumed to be the same $\Gamma = 13.2$ eV (see Table I) and thus are not changing the relative weights. This means for a Q value of $Q = 2.8$ keV the two-hole states seem not to play the dominant role for the determination of the neutrino mass, at least judging from the states of energies closest to the Q values.

Under the assumption, that one resonance determines the upper end of the spectrum at the Q value, one has four parameters to fit simultaneously: the neutrino mass m_ν, the distance of the resonance to the Q value $\Delta E_{f'}$, the strength S, and the width $\Gamma_{f'}$. To include the experimental resolution in the fit, one must fold the experimentally determined profile of the detector into the upper end of the theoretical spectrum.

V. CONCLUSIONS

In the present work the bolometer spectrum after electron capture in ^{163}Ho for the deexcitation of ^{163}Dy has been calculated including the one- and two-hole excitations in Dy. The main improvements compared to Robertson [7] and to Carlson and Nestor [9] are as follows. The two-hole probabilities are calculated in the atoms holmium and dysprosium directly involved in electron capture, by which one wants to determine the neutrino mass. Robertson [7] used for electron capture in $Z = 67$ holmium the results for $Z = 54$ xenon calculated by Carlson and Nestor [9].

The present work also takes into account self-consistently in the relativistic DHF approach the different hole states in ^{163}Dy. So for each one-hole state the remaining 65 electron wave functions are calculated self-consistently and used to determine the two-hole probabilities. The larger number of electrons in Dy than in Xe allows additional two-hole states, which previously have not been included. The two-hole probabilities in Dy calculated here are quite different from the probabilities of Robertson [7] and Carlson and Nestor [9] calculated in $Z = 54$ xenon. To test the numerical results of this work three two-hole probabilities have also been calculated by hand.

The neutrino mass must be determined by a simultaneous fit together with the Q value and the properties of the relevant resonances (assuming a Lorentzian profile, these properties are positions, strengths, and widths), to the upper end of the spectrum. The finite neutrino mass provides at the upper end of the spectrum a characteristic deviation from the usual line shape, which cannot be simulated by a resonance in Dy. This fingerprint close to the Q value should show up in the fit to the data. The finite experimental energy resolution has to be folded into the theoretical spectrum before one fits it to the data. Thus an excellent resolution of the measurement near the Q value is essential.

ACKNOWLEDGMENTS

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