Neutrino mass, electron capture, and the shake-off contributions

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Electron capture can determine the electron neutrino mass, while the β decay of tritium measures the electron antineutrino mass and the neutrinoless double β decay observes the Majorana neutrino mass. In electron capture, e.g., $^{163}_{67}\mathrm{Ho} + e^- \rightarrow {}^{163}_{66}\mathrm{Dy}^* + \nu_e$, one can determine the electron neutrino mass from the upper end of the decay spectrum of the excited Dy, which is given by the Q value minus the neutrino mass. The excitation of Dy is described by one, two, and even three hole excitations limited by the Q value. These states decay by x-ray and Auger electron emissions. The total decay energy is measured in a bolometer. These excitations have been studied by Robertson and by Faessler *et al.* In addition the daughter atom Dy can also be excited by moving in the capture process one (or more) electrons into the continuum. The escape of these continuum electrons is automatically included in the experimental bolometer spectrum. Recently a method developed by Intemann and Pollock was used by DeRujula and Lusignoli for a rough estimate of this shake-off process for "s" wave electrons in capture on ^{163}Ho. The purpose of the present work is to give a more reliable description of "s" wave shake-off in electron capture on holmium. One uses the sudden approximation to calculate the spectrum of the decay of $^{163}_{66}\mathrm{Dy}^*$ after electron capture on $^{163}_{67}$Ho. For that one needs very accurate atomic wave functions of Ho in its ground state and excited atomic wave functions of Dy including a description of the continuum electrons. DeRujula and Lusignoli use screened nonrelativistic Coulomb wave functions for the Ho electrons $3s$ and $4s$ and calculate the Dy* states by first-order perturbation theory based on Ho. In the present approach the wave functions of Ho and Dy* are determined self-consistently with the antisymmetrized relativistic Dirac-Hartree-Fock approach. The relativistic continuum electron wave functions for the ionized Dy* are obtained in the corresponding self-consistent Dirac-Hartree-Fock potential. The result of this improved approach is that shake-off can hardly be seen in the bolometer spectrum after electron capture in ^{163}Ho and thus can probably not affect the determination of the electron neutrino mass.

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I. INTRODUCTION

The absolute values of the neutrino masses are still an open problem. Neutrino oscillations give the differences of the squared neutrino masses but not the absolute value. One hopes within the next years to obtain for the electron antineutrino mass a value or at least a better upper limit in the tritium decay by KATRIN in Karlsruhe [1].

The main aim of the neutrinoless double β decay is to distinguish if neutrinos are of Dirac or Majorana nature and to measure also the effective Majorana neutrino mass [2].

Electron capture for example in holmium can measure the electron neutrino mass [3–6]. In electron capture the upper end of the de-excitation spectrum of Dy at $Q = 2.8$ keV is lowered below Q by the neutrino mass. The sensitivity is increased in the tritium decay and in electron capture by a small Q value:

$$^{163}_{67}\mathrm{Ho} + e^- \rightarrow {}^{163}_{66}\mathrm{Dy}^* + \nu_e. \tag{1}$$

Energy conservation does not allow for $Q = 2.8$ keV to capture electrons from ^{163}Ho$1s_{1/2}$ with 55.618 keV, from $2s_{1/2}$ with 9.394 keV or from $2p_{1/2}$ with 8.918 keV binding energy (see Table I). The first orbital, from which an electron can be captured, is $3s_{1/2}, M1$ with 2.128 keV binding energy.

In the sudden approximation the excitation in Dy* is given by the overlap of holmium, with the hole due to the captured electron, and the complete set of configurations of the daughter $\mathrm{D}'|\mathrm{D}',\mathrm{Dy}\rangle$ in Dy*. The prime indicates, that DHF self-consistent electron orbits of Dy are used to built the Dy* (star indicates an excited state) configurations $|\mathrm{D}'\rangle$. In case of capture from $n\ell_{1/2}$ one has

$$\begin{aligned} 1 &= \langle \mathrm{P},(n,\ell_{1/2})^{-1},\mathrm{Ho}|\mathrm{P},(n,\ell_{1/2})^{-1},\mathrm{Ho}\rangle \\ &= \sum_{D'} \langle \mathrm{P},(n,\ell_{1/2})^{-1},\mathrm{Ho}|\mathrm{D}',\mathrm{Dy}\rangle \langle \mathrm{D}',\mathrm{Dy}|(n,\ell_{1/2})^{-1},\mathrm{Ho}\rangle \\ &= |\langle \mathrm{P},(n,\ell_{1/2})^{-1},\mathrm{Ho}|\mathrm{P}',\mathrm{Dy}\rangle|^2 \\ &\quad + \sum_{D'\neq P'} |\langle \mathrm{P},(n,\ell_{1/2})^{-1},\mathrm{Ho}|\mathrm{D}',\mathrm{Dy}\rangle|^2. \end{aligned} \tag{2}$$

If one uses the Vatai approximation [7,8], setting all single electron overlaps $\langle nlj,\mathrm{Ho}|nlj,\mathrm{Dy}\rangle = 1.0$ apart of the overlap between the captured electron orbital in Ho and the corresponding hole with the same quantum numbers in Dy, Eq. (2)

TABLE I. Important electron binding energies in $^{163}_{67}$Ho [15]. Electrons can only be captured from orbitals overlapping with the nucleus. This restricts capture to $ns_{1/2}$ and in a relativistic treatment to the lower amplitude of $np_{1/2}$. Energy conservation requires, that the Q value $Q = 2.8$ keV must be larger than the binding energy of the electron captured in Ho. This is the case for $3s_{1/2}$ and higher levels.

$n\ell_j$	Notation	E_b[keV]
$1s_{1/2}$	$K1$	55.618
$2s_{1/2}$	$L1$	9.394
$2p_{1/2}$	$L2$	8.918
$3s_{1/2}$	$M1$	2.128
$3p_{1/2}$	$M2$	1.923
$4s_{1/2}$	$N1$	0.4324
$4p_{1/2}$	$N2$	0.3435

reduces to

$$\begin{aligned}&\mathrm{Prob}_{\text{shake-off}}\\&\leqslant [1.0-\langle(n,\ell,j)^{-1},\mathrm{Ho}|(n,\ell,j)^{-1},\mathrm{Dy}\rangle^{(2(2j+1))}]\\&\approx [1.0-0.999^4]=0.004\equiv 0.4\% \end{aligned} \tag{3}$$

with 10% error of the overlap

$$\begin{aligned}&\langle(n,\ell,j)^{-1},\mathrm{Ho}|(n,\ell,j)^{-1},\mathrm{Dy}\rangle\approx 0.9:\\&\mathrm{Prob}_{\text{shake-off}}\leqslant [1.0-0.90^4]\approx 0.34\equiv 34\%,\end{aligned} \tag{4}$$

i.e., 34% of the one-hole states. Since one has only capture from $ns_{1/2}$ and $np_{1/2}$ states with $j = 1/2$ the exponent $2(2j+1)$ is always 4. With electron capture in $n,\ell_{1/2}$,Ho the excited configuration P* (for parent) in Ho has 66 electrons as Dy, but it is not an eigenstate of Dy. The "sum" in Eq. (2) over the daughter configurations D$'$ in Dy represents a sum over the complete set of Dy configurations with excitation energies less than the Q value of 2.8 keV and includes also an integral over the energy of the shake-off continuum states $|E > 0,\mathrm{D}'\ \mathrm{Dy}\rangle$ with E positive. The second term of the last line in Eq. (2) is proportional to the probability to excite in Dy any configuration apart of the configuration P$'$ with a hole in state $|n,\ell_{1/2}\rangle$. This probability includes also the shake-off configurations and allows to estimate a maximal probability for the shake-off process. Thus 0.4% [see Eqs. (2) and (3)] is an upper limit for the shake-off probability relative to the configuration D$'$ with the one-hole in $n,\ell_{1/2}$. With an error of 10% for the overlaps and using the Vatai approximation [7,8], the shake-off can be as strong as 34% of the one-hole states. Without Vatai and 10% error for the single electron overlaps between Ho and Dy, the norm yields no restriction on the shake-off process. In this case shake-off can be as large as the one-hole states. We use the Vatai approximation [7] and [8] for the estimates in Eqs. (2)–(4). For the results in Secs. II to V in this work we do not use this approximation. We calculate all overlaps between Ho and Dy orbits exactly.

The important message from Eqs. (2)–(4) is that a small uncertainty due to approximations for the electron wave functions can with this lever produce a large increase of two orders for the shake-off process. Thus very accurate wave functions are essential:

TABLE II. Overlaps of the $3s$ and $4s$ wave functions in Ho with Dy. The self-consistent relativistic Dirac-Hartree-Fock results are shown in the second column. The fourth column gives the same overlaps calculated with nonrelativistic screened Coulomb waves functions. The effective charges for the nonrelativistic screened Coulomb wave functions are chosen as in the work of DeRujula and Lusignoli $Z_{\text{eff}} = 54.9$ for Ho $3s$ and all electron excited states required by the perturbation based on this hole state and $Z_{\text{eff}} = 43.2$ for Ho $4s$ and all excited electron orbits needed by perturbation. DeRujula and Lusignoli [9] use the perturbation approach of Intemann and Pollock [10] to obtain with $H' = -1/r + \int |\varphi(\vec{r}_1)|^2/|\vec{r}-\vec{r}_1|$ the wave functions in Dy. [In Dy one has one proton less in the nucleus than in Ho and an additional electron hole in the state $\varphi(\vec{r})$.] In our work we calculate the electron wave functions by self-consistent DHF. For the numbers given in columns four and five of this table the Dy wave functions are directly calculated as nonrelativistic Coulomb waves.

	DHF	$1-\langle\text{DHF}\rangle^4$	Coul.	$1-\langle\text{Coul.}\rangle^4$
$\langle 3s,\mathrm{Ho}\|3s,\mathrm{Dy}\rangle$	0.99940	0.00239	0.99932	0.00271
$\langle 4s,\mathrm{Ho}\|4s,\mathrm{Dy}\rangle$	0.99909	0.00363	0.99848	0.00607
$\langle 3s,\mathrm{Ho}\|4s,\mathrm{Dy}\rangle$	−0.01982	–	0.56828	–
$\langle 4s,\mathrm{Ho}\|3s,\mathrm{Dy}\rangle$	0.02067	–	0.56817	–
$\langle 3s,\mathrm{Ho}\|4s,\mathrm{Ho}\rangle$	0.0	–	0.56857	–
$\langle 3s,\mathrm{Dy}\|4s,\mathrm{Dy}\rangle$	0.0	–	0.56952	–

$$H'(r) = +1/r - \int d^3r_1\ |\varphi_{3s/4s}(\vec{r}_1)|^2/|\vec{r}-\vec{r}_1|, \tag{5}$$

$$V(r) = -(Z_{\text{eff}}-1)/r - \int d^3r_1\ |\varphi_{3s/4s}(\vec{r}_1)|^2/|\vec{r}-\vec{r}_1|. \tag{6}$$

The relativistic self-consistent electron orbitals for Dy [12–14] yield for shake-off a much smaller probability than Ref. [9], which determines the Dy orbitals by perturbation $H'(r)$ (5) based on Ho (see Fig. 1) as in Ref. [10]. Since the overlap between the corresponding Ho and Dy functions is practically 100% (see Table II) the error due to first order perturbation can only reduce the overlap. If the error of the overlaps is, e.g., 10% the probability for two-hole states including shake-off is $1.0–0.9^4 = 0.34$. This probability of 34% is according to Table II by a about two orders larger than the correct value of about 0.4%. This can explain the large results for shake-off of Ref. [9]. These upper limits for shake-off (2)–(4) are calculated with the Vatai approximation [7,8].

The improvements compared to [9,10] are:

(i) The sudden approximation [6,16–18] with self-consistent Dirac-Hartree-Fock (DHF) wave functions for the Dy atom is used to determine the electron capture probability and not the less reliable first order perturbation theory [9,10].

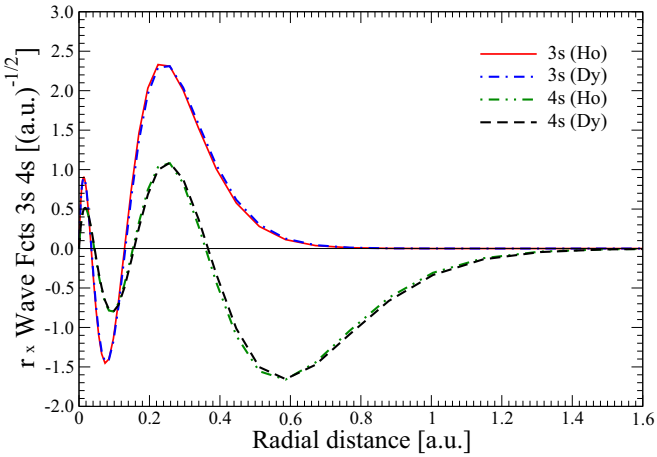

FIG. 1. Nonrelativistic Coulomb wave functions $3s$ (solid), $4s$ (dashed-dot-dot) in Ho with the effective charges chosen by DeRujula and Lusignoli [9] $Z_{\rm eff}(3s) = 54.9$ and $Z_{\rm eff}(4s) = 43.2$. In Ref. [9] the s-wave functions for Dy including the continuum are calculated according to [10] in first order with the perturbation (5). But for this figure the screened nonrelativistic "Coulomb" wave functions for ^{163}Dy are calculated exactly [11] and not with first order perturbation relative to Ho as in Ref. [9], for the potential (6) with a $3s$ or $4s$ hole in Dy. The charge of the nucleus is reduced by one from Ho to Dy, but the electron hole in Dy in the orbit $3s$ (dashed-dot) or $4s$ (dashed) increases for the outer electrons the charge again effectively by one. The change from Ho to Dy is almost not visible in the wave function of this figure. The hole state has in Dy the effect to smear out the positive charge of the nucleus compared to Ho and increases by that effectively the nuclear radius. Thus the effect is to shift the functions in Dy slightly to the right to larger radial distances. This small change of the wave function from Ho to Dy restricts in the sudden approximation using the Vatai approximation [7,8] the probability for two-hole states including also shake-off to the very small values 0.00271 for $3s$ and 0.00607 (see Table II) for $4s$ in column five of Table II. These small probabilities for two-hole states including shake-off agrees qualitatively with the more reliable self-consistent relativistic Dirac-Hartree-Fock [12] result of column three in Table II. This shows, that shake-off can have only a very minor effect on the bolometer spectrum of the Dy decay after capture in Ho.

(ii) The electron wave functions in $^{163}_{67}$Ho are not given as nonrelativistic screened Coulomb functions, but are calculated with the relativistic, self-consistent Dirac-Hartree-Fock approach [12–14] with full antisymmetrization. Among many other advantages the electron orbitals are in this way all orthogonal (see Table II).

(iii) The wave function of the bound electrons in Dysprosium are again determined self-consistent and relativistic by Dirac-Hartree-Fock [12–14] even allowing for $3s$ and $4s$ hole states for the determination of the self-consistent wave functions. In Refs. [9,10] the electron orbitals for the daughter Dy are calculated in first-order perturbation theory (5).

(iv) The s-wave function for the 66th continuum electron for shake-off in Dy is calculated relativistically in the self-consistent DHF potential of the 65 electrons in ionized Dy under the condition that the continuum s orbitals are orthogonal in the bound s orbits in Dy.

(v) The problem of the numerical stability is tested carefully. For the continuum electron wave functions in Dy for the radial coordinate 250 up to more than 700 mesh points were used depending on the energy. The integration over the continuum electron energies for the shake-off electron are performed from 0 to $Q = 2.8$ [keV] with 417 mesh points. Integrations for the norms, the overlaps and the integration over the shake-off in the continuum were done in parallel with the Trapez rule (error $\propto$ second derivative), the Kepler-Simpson rule (error $\propto$ fourth derivative), the Bode-Boole rule (error $\propto$ sixth derivative), and the Weddle rule. From the points of stability and accuracy the Bode-Boole's rule turned out to be the most reliable. All the calculations were done in double precision.

(vi) The DHF overlaps of $\langle 3s,\mathrm{Ho}|3s,\mathrm{Dy}\rangle = 0.99940$ and $\langle 4s,\mathrm{Ho}|4s,\mathrm{Dy}\rangle = 0.99909$ limit in the Vatai approximation [7,8] the two-hole probability including the shake-off process, which requires a second hole, to 0.24% and 0.36% of the one-hole excitations. An error of 10% in calculating the single orbital overlaps between Ho and Dy due to first order perturbation theory [9,10] estimated again with Vatai can increase the shake-off probability by two orders of magnitude. Equation (2) serves as lever to produce from a small uncertainty of the single electron overlaps a large increase of the shake-off probability. If one does not use the Vatai approximation and puts all electron orbital overlaps of Ho with Dy to 0.999, the definite upper limit (including one- and two-hole and shake-off excitations) for shake-off is 12% relative to the one-hole states. The norm gives without Vatai no restriction for the shake-off with an error of 10% for the $\langle n,\ell,j,\mathrm{Ho}|n,\ell,j,\mathrm{Dy}\rangle$ single electron overlaps.

(vii) In this work the different one-hole, two-hole, and shake-off contributions are taken from the theory without adjusting them in different ways to fit the experiment. In Ref. [9] the authors write on the second page in the right column: "Our estimate of the height of the N1(4s)O1(5s) shakeup peak is a factor $\approx$2.5 too low. It is possible to correct in similarly moderate ways the other contributions such as to agree with the data."

II. ELECTRON CAPTURE WITH SHAKE-OFF

The de-excitation spectrum of the daughter ^{163}Dy* after electron capture in ^{163}Ho is described in Refs. [3,6] assuming Lorentzian line profiles by the expression:

$$\frac{d\Gamma}{dE_c} \propto \sum_{i=1,\ldots N_\nu} |U_{e,i}|^2 (Q-E_c)\sqrt{(Q-E_c)^2 - m_{\nu,i}^2} \left(\sum_{f=f'} \lambda_0 B_f \frac{\Gamma_{f'}}{2\pi} \frac{1}{(E_c - E_{f'})^2 + \Gamma_{f'}^2/4} \right.$$
$$+ \sum_{f=f';p'\langle F;q_b'\rangle F} \lambda_0 B_{f,p'\langle F;q_b'\rangle F} \frac{\Gamma_{f',p'}}{2\pi} \frac{1}{(E_c - E_{f',p'})^2 + \Gamma_{f',p'}^2/4}$$
$$\left. + \int dk_{q'} \lambda_0 B_{f,p'\langle F;q_c'\rangle 0} \frac{\Gamma_{f',p',q'}}{2\pi} \frac{1}{(E_c - E_{f',p',q'})^2 + \Gamma_{f',p',q'}^2/4} \right). \quad (7)$$

The factor in front of the brackets originates from the phase space of the neutrino. It is the same as for the single β decay. The three terms in the three lines in Eq. (7) in the brackets describe the decay of of the excited daughter Dy from one-hole f' excitations, from two-hole excitations f', p' with a shake-up of p' to q' into a bound orbit and the excitation of two-holes f', p' with one electron p' moved to q' into the continuum with an energy $E > 0$ (shake-off). The integration over the wave number $k_{q'}$ yields for shake-off a dimensionless strength factor $dk_{q'} \cdot B_{f',p'\langle F,q'\rangle o}$ and thus has the same dimension as the other strength factors $B_{f'}$ and $B_{f',p'\langle F,q'\rangle F}$. The transformation from an integral over the wave number to an integral over the energy yields nonrelativistically a factor $1/(2 \cdot \pi \cdot k_{q'})$. [For the relativistic expression used here see Eq. (22)]. $U_{e,i}^2$ is the probability for the admixture of different neutrino mass "i" eigenstates into the electron neutrino "e" flavor eigenstate. For the Q value we take $Q = (2.8 \pm 0.08)$ [keV] from the ECHo collaboration [4,19–22], while the recommended value [23] $Q = (2.55 \pm 0.016)$ keV seems to be to small. E_c is the excitation energy of final dysprosium. The energy difference $Q - E_c$ is carried away by the neutrino. $B_f, B_{f,p'\langle F;q_b'\rangle F}$, and $B_{f,p'\langle F;q_c'\rangle 0}$ are the overlap and exchange corrections for the one-hole, the bound two-hole, and the shake-off two-hole states. λ_0 contains the nuclear matrix element squared [16]. Since λ_0 is here not calculated the theoretical results are given in arbitrary units fitted to the $N1$, $4s_{1/2}$ experimental peak. $E_{f'}, E_{f',p'}$, and $E_{f',p';q'>0}$ are the one-hole, the two-hole shake-up, and the two-hole shake-off excitation energies in dysprosium (see Tables I and III). $\Gamma_{f'}, \Gamma_{f',p'}$, and $\Gamma_{f',p';q'>0}$ are the widths of the one- and two-hole states and the two-hole states with shake-off in dysprosium [6,18]. If the escape width of the electron in the continuum is included, it has to be added to $\Gamma_{f',p';q'>0}$ in line 3 of Eq. (7). The escape width of the electron from the shake-off state is neglected here and in Ref. [9]. This additional escape contribution to the width should be studied in the future. It could smear out the shake-off contributions as function of the energy. The difference between the emitted neutrino and the escape electron is that event by event the energy of the electron (plus the two-hole binding energy) is measured in the bolometer. The neutrino escapes undetected. Here as in all other calculations for the de-excitation of Dy after electron capture a Lorentzian shape is assumed. This is probably a good description. Holmium is in the ECHo experiment built in a gold film positioned as an interstitial or it occupies a position of 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 since the shape of the resonance lines are important for the determination of the neutrino mass, this assumption must be studied in the future more carefully. For the neutrino mass determination the highest two-hole state with an energy 2.474 keV [6,24] is the most important excitation. (2.0418 keV $3s$ in Dy plus 0.4324 keV $4s$ from Ho. Due to the hole in Dy the second hole should "see" an effective nuclear charge similar as in Ho.) We describe the atomic wave function by a single Dirac-Hartree-Fock Slater determinant. The one-hole B_f' and the bound two-hole probabilities (shake-up) $B_{f',p';q'}$ are derived in Refs. [2,6,18]. We concentrate here only on the shake-off probability $B_{f',p';q'>0}$ with the electron q' in the continuum. The antisymmetrized Slater determinants for the wave functions of the initial holmium in the ground state $|G\rangle$ and the excited one electron hole states $|A_{f'}'\rangle$ in dysprosium read in second quantization:

$$|G\rangle = a_1^\dagger a_2^\dagger a_3^\dagger \cdots a_Z^\dagger |0\rangle, \quad (8)$$
$$|A_{f'}'\rangle = a_1'^\dagger a_2'^\dagger \cdots a_{f'-1}'^\dagger a_{f'+1}'^\dagger \cdots a_Z'^\dagger |0\rangle. \quad (9)$$

The antisymmetrized two-hole state in Dy with shake-off is

$$|A'_{p',f':q'>0}\rangle = a_1'^\dagger a_2'^\dagger \cdots a_{f'-1}'^\dagger a_{f'+1}'^\dagger \cdots a_{p'-1}'^\dagger a_{p'+1}'^\dagger \cdots a_Z'^\dagger a_{q'>0}'^\dagger |0\rangle. \quad (10)$$

TABLE III. Electron binding energies and width of two-hole states in $^{163}_{66}$Dy, which contribute to s-wave shake-off. Energy conservation requires, that the Q value $Q = 2.8$ keV must be larger than the two-hole binding energy plus the energy of the electron in the continuum. The shake-off contributions for the two-hole states start at the two-hole binding energy in the bolometer spectrum as a function of E_c. The width includes only the contribution from the decay of the two-hole states, but not the escape width of the continuum electron.

$n_1\ell_{j,1}, n_2\ell_{j,2}$	two-hole E_b [keV]	Width [keV]
$3s_{1/2}, 4s_{1/2}$	2.4742	0.0264
$4s_{1/2}, 4s_{1/2}$	0.8414	0.0108
$4s_{1/2}, 5s_{1/2}$	0.4583	0.0107
$4s_{1/2}, 3p_{1/2}$	2.2692	0.0114
$5s_{1/2}, 3p_{1/2}$	1.8861	0.0114
$3s_{1/2}, 4p_{1/2}$	2.3853	0.0186
$4s_{1/2}, 4p_{1/2}$	0.7525	0.0107
$5s_{1/2}, 4p_{1/2}$	0.3776	0.0106

TABLE IV. Overlaps of ^{163}Ho electron orbits with bound and continuum wave functions (19) $P_k(r)$ and $Q_k(r)$ in ^{163}Dy. The continuum wave functions are normalized asymptotically as in Eq. (18) to the δ function for the wave numbers (19). For the integral over the continuum energy one has to square the overlaps of Ho functions with the continuum in Dy and to change to the energy normalization [see after Eq. (22)]. This transformation squared gives roughly a factor: $1/(2\pi k) \approx 0.014$ [a.u.] for an electron energy of 1.768 keV in the Dy continuum. On the other side the transformation from the δ function of energies in Hartree to energies in keV increases shake-off result by a factor 36.7498 [Hartree/keV].

	$\|3s,\mathrm{Dy}\rangle$	$\|4s,\mathrm{Dy}\rangle$	$\|5s,\mathrm{Dy}\rangle$
$\langle 3s,\mathrm{Ho}\|$	0.9940	-1.98226×10^{-2}	6.20190×10^{-3}
$\langle 4s,\mathrm{Ho}\|$	2.06722×10^{-2}	0.99909	-1.87503×10^{-2}
$\langle 5s,\mathrm{Ho}\|$	-6.31396×10^{-3}	1.97766×10^{-2}	0.99928
	$\|E = 0.884\ \mathrm{keV},s,\mathrm{Dy}\rangle$	$\|E = 1.768\ \mathrm{keV},s,\mathrm{Dy}\rangle$	$\|E = 2.653\ \mathrm{keV},s,\mathrm{Dy}\rangle$
$\langle 3s,\mathrm{Ho}\|$	1.383×10^{-2}	1.044×10^{-2}	8.314×10^{-3}
$\langle 4s,\mathrm{Ho}\|$	-1.407×10^{-2}	-7.366×10^{-3}	-4.881×10^{-3}
$\langle 5s,\mathrm{Ho}\|$	4.926×10^{-3}	2.095×10^{-3}	1.329×10^{-3}

The probability to form a two-hole shake-off state is proportional to

$$P_{f',p';q'>0} = |\langle A'_{f',p';q'}|a_i|G\rangle|^2. \tag{11}$$

The relative shake-off probability normalized to the $3s$ one-hole excitation is

$$B_{f',p';q'>0} = \frac{|\psi_f(R)\langle A'_{f',p':q'<0}|a_f|G\rangle|^2}{|\psi_{3s1/2}(R)|^2} = P_{f',p';q'>0} \cdot \frac{|\psi_f(R)|^2}{|\psi_{3s1/2}(R)|^2}. \tag{12}$$

Normally the wave function of the captured Ho electron is taken for the nuclear matrix element at the origin. Here we take this electron wave function at the nuclear radius. Due to the weight r^2 of the integration this is a better choice with

$$\begin{aligned} &P_{f',p';q'>0} \\ &= |\langle 0|a'_{q'}a'_Z...a'_{p'+1}a'_{p'-1}...a'_{f'+1}a'_{f'-1}...a'_{1'}a_f a_1^+...a_Z^+|0\rangle|^2 \\ &= |\langle A'_{p',f'\langle F;q'\rangle F}(2\ \mathrm{holes})|a_f|G\rangle|^2 \\ &\approx \left|\langle q'_{>0}|p_{<F}\rangle \prod_{k=1..Z\neq f,p} \langle k'|k\rangle\right|^2. \end{aligned} \tag{13}$$

q' is for the shake-off a continuum 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, j in the parent k, f, p and the daughter atom k', f', 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 and p. q' is for the shake-off contribution a continuum state in Dy. In the Vatai approximation [7,8] (not used here) one replaces the product over k in Eq. (14) by unity. Because now a squared "nondiagonal" overlap is involved in Eq. (13) with $|\langle q'_{Dy}|p_{\mathrm{Ho}}\rangle|^2$, the two-hole shake-up and shake-off contributions are reduced by a "nondiagonal" overlap squared. If one exchanges the states f' and p', one obtains an additional "−" sign. But since one has to square the expression, a phase is irrelevant.

To evaluate the probability for the shake-off process one integrates over the wave numbers $k_{q'}$ or the the excitation energy of the continuum states q' with the same orbital ℓ and total j angular momentum as the state p Eq. (7). Here the excitations are restricted to s waves:

$$P_{f',p'} = \sum_{q'>F} |\langle p_{<F,\mathrm{Ho}}|q'_{>F,\mathrm{Dy}}\rangle\langle q'_{>F,\mathrm{Dy}}|p_{<F,\mathrm{Ho}}\rangle| \times \prod_{k=k'<F_{\mathrm{Dy}}\neq f,p} |\langle k'_{\mathrm{Dy}}|k_{\mathrm{Ho}}\rangle|^2. \tag{14}$$

In the Vatai approximation [7,8] not used in this work the overlaps $\langle k'_{\mathrm{Dy}}|k_{\mathrm{Ho}}\rangle \approx 0.999$ are put to unity. We calculate all overlaps $\langle k'_{\mathrm{Dy}}|k_{\mathrm{Ho}}\rangle$ exactly with self-consistent, relativistic Dirac-Hartree-Fock electron wave functions.

III. THE DY CONTINUUM WAVE FUNCTIONS

To obtain the correct continuum wave functions for the shake-off electron in Dy one has three problems:

(1) One needs a potential for this electron. This can be derived from the self-consistent Dirac-Hartree-Fock electron wave functions in Dy taking into account the Coulomb field of the 66 protons in the nucleus and the 65 bound electrons allowing for the different empty states (see Fig. 3). Fig. 3 shows an analytic approximation to the local part of the Z-1 selfconsistent potential of Dy. Fig. 4 shows local potential approximants to different hole configurations in Dy.

(2) With this potential the relativistic continuum electron wave functions have to be calculated with the condition, that these states are orthogonal to all bound orbits in Dy. For calculating the relativistic wave functions in this potential we take the code of Salvat *et al.* [11] together with Schmidt orthogonalization. If the continuum waves are calculated with the nonlocal DHF potential, they are automatically orthogonal to the bound states like the bound orbitals among each other. Since we approximate the potential for the continuum by the local approximation (15), (17) in Figs. 3 and 4, we have to Schmidt orthogonalize the continuum wave functions (see Fig. 5).

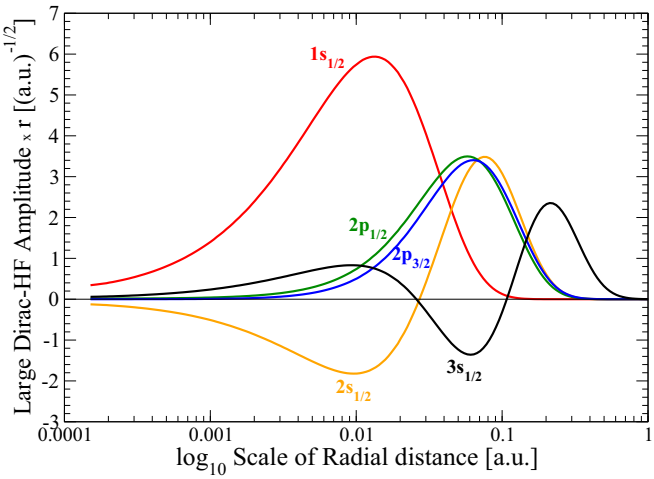

FIG. 2. Large amplitudes $P(\vec{r})$ for $1s$, $2s$, $2p_{1/2}$, $2p_{3/2}$, and $3s$ Dy electrons normalized DHF wave functions in atomic units for the the radial distance (Bohr radii) and (atomic units)$^{-1/2}$ for the wave functions.

(3) The wave functions of Salvat *et al.* [11] are normalized to δ functions in wave numbers $2\pi\delta(k-k')$. For the integration over the excitation energy in the continuum (7) the wave functions have to be normalized to energy δ functions $\delta(E-E')$ (see Fig. 6).

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

$$V_{\text{shake-off}}(r) = \frac{-66}{r} + \sum_{k \text{ occupied } e} g'_k \int d^3\vec{r}\,\frac{|\varphi_k(\vec{r}')|^2}{|\vec{r}-\vec{r}'|}. \quad (15)$$

$g'_k s$ are the number of bound electrons in the self-consistent occupied orbits $|k\rangle = |n,\ell,j\rangle$ of Dy. To determine the potential for the shake-off electrons in Dy one needs the occupied self-consistent Dirac-Hartree-Fock orbitals $P_k(r)$ and $Q_k(r)$ [as examples for $P(r)$ see Fig. 2]:

$$\varphi_k(\vec{r})r = (P_k(\vec{r}); Q_k(\vec{r})), \quad (16)$$

$$V_{\text{shake-off}} \approx -\frac{66}{r} + \frac{65}{r}(1-e^{-ar}). \quad (17)$$

We adjust an analytic expression (17) to the DHF potential (see Fig. 3). At small r one obtains the Coulomb potential of the Dy nucleus $-66/r$ and for large r the dependence $-1/r$ of the ionized Dy. With the help of Eqs. (15) and (17), and Fig. 3 one can determine the only free parameter "a[1/(length = a.u.)]" as $a = 3.4$. The self-consistent Dy potential with 66 electron is shown in Fig. 4 for the Dy ground state and for a hole in $3s$ and $4s$ in Dy.

The Relativistic continuum wave functions in the potential (17) are determined with the code of Salvat, Fernandes-Varea, and Williamson [11] (see Fig. 5). This code can handle potentials with the properties $\lim_{r\to\infty} rV(r) = \text{constant}$. All our potentials are of this nature. The wave functions are normalized with the WKB approximation to

$$\lim_{r\to\infty} P_k(r) = 2\sin\left(kr - \ell\frac{\pi}{2} - \eta\ln(2kr) + \Delta + \delta\right). \quad (18)$$

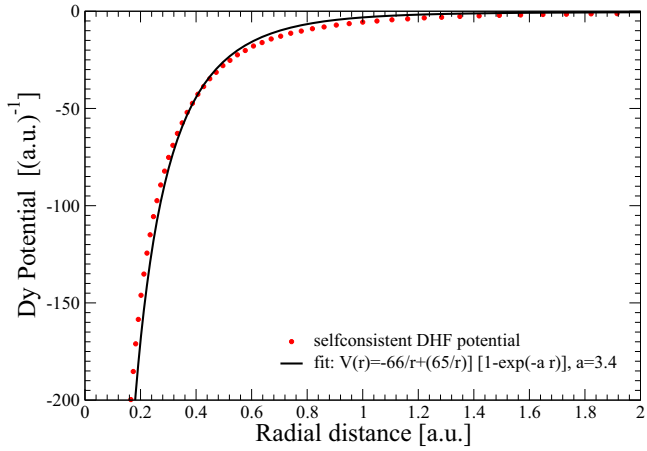

FIG. 3. Self-consistent DHF potential [dotted; dimension: 1/(length = a.u.)] and analytic approximation (solid) with a = 3.4. [see Eqs. (15) and (17).]

For $Q(r)$ one has a similar asymptotic expression. The problem of the normalization of the continuum Dirac wave function is for example discussed by Rose in his book *Relativistic Electron Theory* [25] or by Walter Greiner in the book on "Relativistic Quantum Mechanics" [26]. The normalization is also discussed by Goldberg *et al.* [27], and by Perger and Karighattam [28] on their p. 394. We follow here this recommendation [28]. In the asymptotic expression (18) η is the Sommerfeld parameter, Δ the Coulomb phase shift, and δ takes into account deviations from a pure Coulomb potential. The usual way [28] to determine the norm is to normalize only $P(r)$ to the δ function in wave numbers or energies and treat the small relativistic amplitude in the same way. Since the electron energies required for shake-off in the continuum are small compared to the electron rest mass $m_e c^2 = 510.9989$ keV this often used normalization should be good for our purpose.

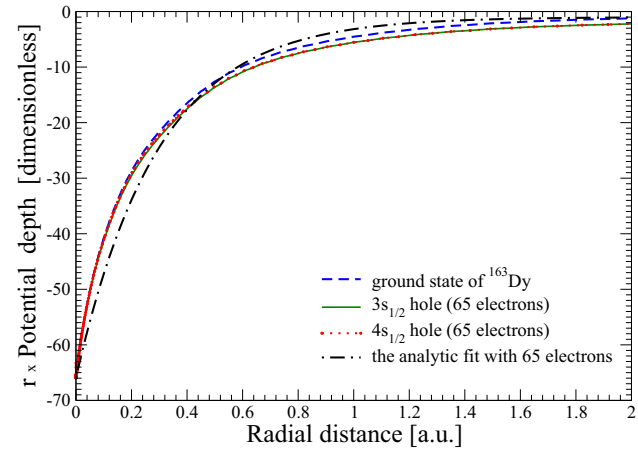

FIG. 4. Radial distance r times the self-consistent potential [dimensionless] for the ground state of the Dy atom with 66 electrons (dashed), r times the self-consistent potential with a hole in $3s$ and 65 electrons (solid), r times the self-consistent potential with a hole in $4s$ and 65 electrons (dotted), and r times the analytical fit to the ground state potential (17) (dashed-dot lines).

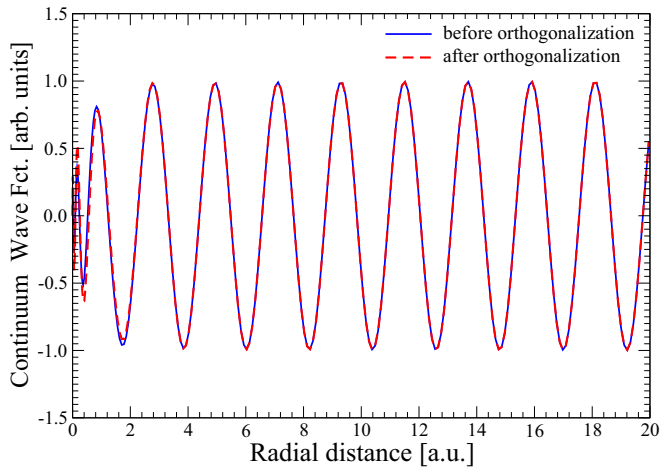

FIG. 5. Large amplitude $P(r)$ of the s wave at $E = 4$ [Hartree] $\equiv 108.8$ [eV] before (solid) and after Schmidt orthogonalization (dashed).

The electron energy in the continuum can be due to energy conservation not larger than the Q value of 2.8 keV minus the excitation energy of the two-hole state. So for shake-off with capture from $3s$ the energy of the electron in the continuum must be less than 0.758 keV (extreme nonrelativistic). The most important second hole is $4s1/2$ and thus for the two holes in $3s$ and $4s$ the integration over the shake-off electrons is restricted to 2.800–2.474 keV = 0.236 keV. For capture from the two $4s1/2$ states the binding energy limits the integration in Eq. (7) to an upper limit of 2.800–0.841 = 1.959 keV.

The asymptotic (18) requirement normalizes the asymptotic form of $P(r)$ with $\lim_{r\to\infty} P_k(r)$ to the δ function in wave numbers. Continuum wave functions for different electron energies are orthogonal. The δ function strength is determined by the asymptotic, which yields infinity for the norm integration. Thus for continuum wave functions (18) calculated with the DHF self-consistent local potentials (15) and (17) is also normalized in the wave numbers to $2\pi\delta(k-k')$ and in the energy to $\delta(E-E')$. The Schmidt orthogonalization does not change this, since it modifies the wave functions only at short distances and the δ function is determined by the asymptotic. Comparing the two asymptotic forms gives us the transformation factor from the wave number $2\pi\delta(k-k')$ to the energy δ function $\delta(E-E')$ normalization:

$$\int_{r=0}^{\infty} dr 2\sin\left(kr - \ell\frac{\pi}{2} - \eta\ln(2kr) + \Delta + \delta\right) \times 2\sin\left(k'r - \ell\frac{\pi}{2} - \eta\ln(2kr) + \Delta + \delta\right) \approx 2\pi\delta(k-k'). \quad (19)$$

The wave number is connected with the relativistic and nonrelativistic energies by the equations

$$E_{\rm rel}^2 = c^2\hbar^2k^2 + m^2c^4 \to c^2k^2 + c^4 \text{ (in atomic units)},$$
$$E_{n-\rm rel} = \frac{1}{2}k^2, \quad k = \alpha\sqrt{E_{n-\rm rel}(E_{n-\rm rel} + 2\cdot c^2)} \quad (20)$$

with $c = 1/\alpha = 137.035999$ in [atomic units]. We use to change from the asymptotic wave number normalization $2\pi\delta(k-k')$ to the normalization $\delta(E-E')$ well known relations for Dirac δ functions given for example in Landau-Lifschitz [29] (Vol. 3, Chaps. 5 and 33):

$$\delta(g(x)) = \frac{\delta(x-x_0)}{|g'(x_0)|}, \quad \delta(ax) = \frac{1}{|a|}\delta(x) \quad (21)$$

with $g(x_0) = 0$. The transformation from the asymptotic wave number normalization $P_k(r)$ to the asymptotic energy δ function normalization is

$$P_E(r) = P_k(r)\sqrt{\frac{1}{2\pi}\frac{1}{c}\frac{\sqrt{k^2+c^2}}{k}} \approx P_k(r)\frac{1}{\sqrt{2\pi k}}$$
$$\delta(E[\text{Hartree}]) = \delta(36.74932386E[\text{keV}]) = 0.027121138506\delta(E[\text{keV}]). \quad (22)$$

We transform the $Q_k(r)$ in the same way using the asymptotic expression to obtain the transformation factor. For shake-off one has to calculate the overlap of the bound Ho electron orbitals $|p\rangle$ with the continuum wave functions in Dy $|q'\rangle$, i.e., $\langle q'_{>0}|p_{<F}\rangle$ Eq. (13) (see Fig. 6). For this one expands the configuration of Ho after capture of the bound electron $|P,(b)^{-1},\text{Ho}\rangle$ with now the same number of protons as Dy (but not a Dy eigenstate) into the complete set of configurations

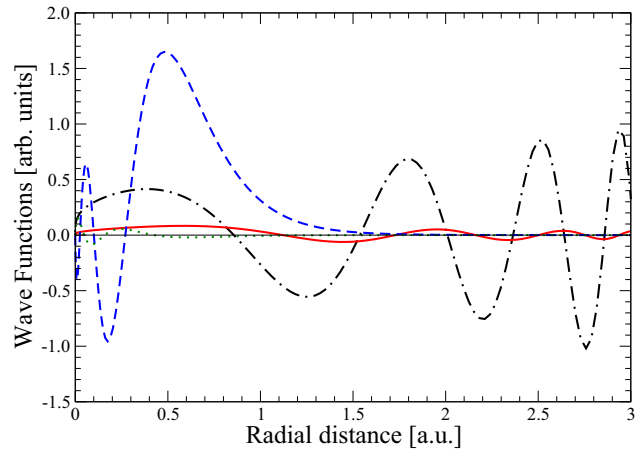

FIG. 6. Wave function $P(r)$ (dashed-dot line) and $Q(r)$ (solid line) Eq. (16) in the Dy continuum at 50 [Hartree] = 1.36 keV. The continuum wave functions P and Q are normalized to $\int dr[P(r)^2 + Q(r)^2\ ] = 2\pi\delta(k-k')$. The $4s$ bound state in Ho is normalized to unity [dashed for $P(r)$ and dotted for $Q(r)$]: $\int dr[P(r)^2 + Q(r)^2] = 1$. The overlap $\langle ns,\text{Ho}|\text{E},s,\text{Dy}\rangle$ squared is proportional to the shake-off process as a function of energy. The continuum wave functions P_E and Q_E are dimensionless, while the bound states $P_{4s}(r)$ and $Q_{4s}(r)$ are in atomic units [(a.u.)$^{-1/2}$].

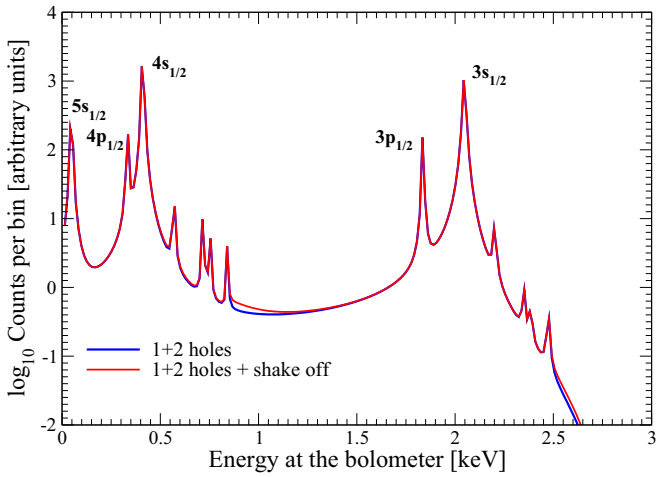

FIG. 7. Theoretical results in arbitrary units of the sum of the one- and two-hole de-excitations compared to the sum of the one-, two-hole, and the shake-off de-excitation as measured by the bolometer spectrum (7). The arbitrary units are adjusted to the experimental $N1$, $4s_{1/2}$ one-hole peak. The nature of the one hole states are indicated. The two-hole peaks are by about two orders of magnitudes smaller than the one hole peaks. Shake-off can almost not been seen.

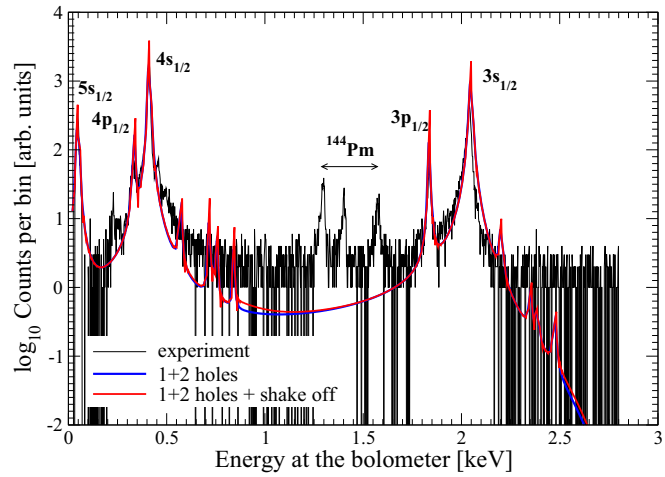

FIG. 8. Experimental and theoretical results of the sum of the one- and two-hole de-excitations (dashed line) and the sum of the one-, two-hole, and the shake-off de-excitation (solid line) for the bolometer spectrum (7). The experimental data are from the ECHo collaboration [4,21]. The two theoretical spectra are adjusted to experiment at the $N1$, $4s_{1/2}$ peak. The nature of the one-hole states are indicated. The two-hole peaks are by about two orders of magnitudes smaller than the one-hole peaks. The shake off contributions can hardly been seen in this scale. Some bins contain no experimental counts, thus the $\log_{10}$ for these experimental values are minus infinity. To fit the 1931 experimental points for the bolometer energy of 0.0 to 2.8 keV, the theoretical spectrum of 200 mesh points had to be interpolated to the data points for this figure. Figure 7 contains the 200 original theoretical results without interpolation for the bolometer spectrum over E_c between 0.0 and 2.8 keV. The interpolation is normally very good (compare Figs. 7 and 8) but difficult at some sharp minima and maxima.

$|D,\mathrm{Dy}\rangle$ in Dy including the continuum:

$$
\begin{aligned}
|P,(b)^{-1},\mathrm{Ho}\rangle &= \sum_{D\neq P,\mathrm{bound}} a_D|\mathrm{D},\mathrm{Dy}\rangle \\
&\quad + \int_0^\infty dE' a(\mathrm{D},E')|\mathrm{D},E',\mathrm{Dy}\rangle, \\
a_D &= \langle \mathrm{D},\mathrm{Dy}|\mathrm{P},(b)^{-1},\mathrm{Ho}\rangle, \\
a(\mathrm{D},E'') &= \langle \mathrm{D},E'',\mathrm{Dy}|\mathrm{P},(b)^{-1},\mathrm{Ho}\rangle \\
&= \int_0^\infty dE' a(\mathrm{D},E')\langle \mathrm{D},E'',\mathrm{Dy}|\mathrm{D},E',\mathrm{Dy}\rangle.
\end{aligned}
\tag{23}
$$

Here, the δ-function normalization of the continuum wave functions in Dy is used: $\langle E'',\mathrm{Dy}|E',\mathrm{Dy}\rangle = \delta(E''-E')$. The probability forming a specific hole state $|k',\mathrm{Dy}\rangle$ in Dy in a bound orbit after capture of the electron $|P,(b)^{-1},\mathrm{Ho}\rangle$ is proportional to $|\langle k',\mathrm{Dy}|b,\mathrm{Ho}\rangle|^2$ and and for the continuum $|E'',\mathrm{Dy}\rangle$ to $|\langle E'',\mathrm{Dy}|b,\mathrm{Ho}\rangle|^2$ integrated over the continuum energy of the shake-off electron E''.

IV. RESULTS FOR SHAKE-OFF

To calculate the shake-off contributions, one has to determine first the overlap between the bound Ho states $ns_{1/2}$ and in principle also $np_{1/2}$ with $n \geqslant 3$ and the continuum wave functions in Dy. Since we restrict this work to s-wave shake-off we need only the overlaps $\langle n \geqslant 3,s_{1/2},\mathrm{Ho}|E,s,\mathrm{Dy}\rangle$. In the summed spectrum with one-hole, two-hole, and shake-off in Figs. 7 and 8 the shake-off contribution is hardly visible. Here and also in Ref. [9] only the decay width of the two-hole states are included. Three hole states can be neglected [9]. The electron in the continuum has an escape width, which is not included.

Figure 7 shows the logarithmic spectrum of the one-hole, the two-hole, and the s-wave shake-off contributions. The shake-off contributions (see Figs. 9 and 10) are calculated for the different two-hole states listed in Table III. The two-hole spectrum is about two orders of magnitude smaller than the one-hole states. The shake-off spectrum (see Figs. 9 and 10) can hardly be seen on this scale in the total spectrum. Compared to the one-hole peaks it is at least two orders smaller. The integration over the continuum electron energy (7) is done by the Bode method using 417 mesh points. Shake-off is proportional to the square of the overlap $\langle$Ho-bound|Dy-continuum$\rangle$. The two-hole states contributing to s-wave shake-off are listed in Table III. The shake-off contributions (see Fig. 9) of the two-hole states as function of the bolometer energy E_c is starting from the two-hole binding energy up (see Table III). The two main contributions originate from $4s_{1/2},5s_{1/2}$ starting at 0.4583 keV and from $4s_{1/2},4s_{1/2}$ starting at 0.8414 keV (see Tables III and IV). The $\log_{10}$ contributions from $3s_{1/2},4p_{1/2}$ starting at 2.33853 keV (see Table III) are extremely small. The energy difference $Q-E_c$ is carried away by the neutrino and and does not show in the bolometer.

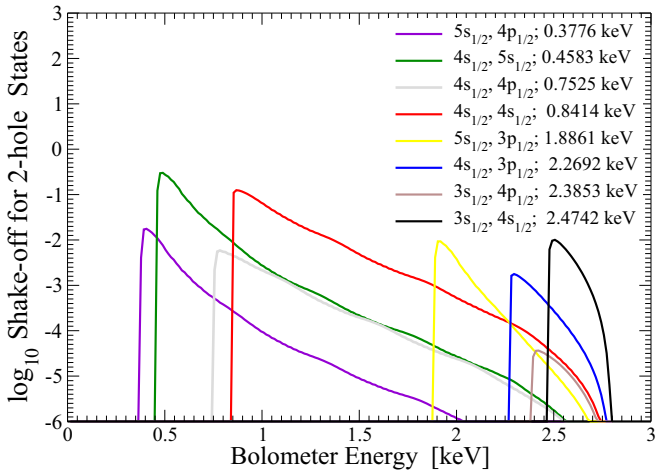

FIG. 9. Shake-off contributions for different two-hole excitations in Dy normalized for the experimental bolometer spectrum (see Fig. 8) to the $N1,4s_{1/2}$ peak. Increasing the energy E_c of the bolometer spectrum the Q value = 2.8 keV is first used to excite the two-hole state. So the shake-off contribution for the bolometer spectrum starts as function of E_c with the two-hole binding energy. Energy conservation yields an upper limit of $Q = 2.8$ keV for the bolometer spectrum. To integrate over the continuum energy of the shake-off electron (7) we divided the interval $\langle 0.0,2.8\rangle$ keV into 417 mesh points. From the left to the right with increasing bolometer energy E_c the start of the different shake-off contributions are indicated in the figure. The energy difference between Q and E_c is carried away by the neutrino, which cannot contribute to the bolometer spectrum.

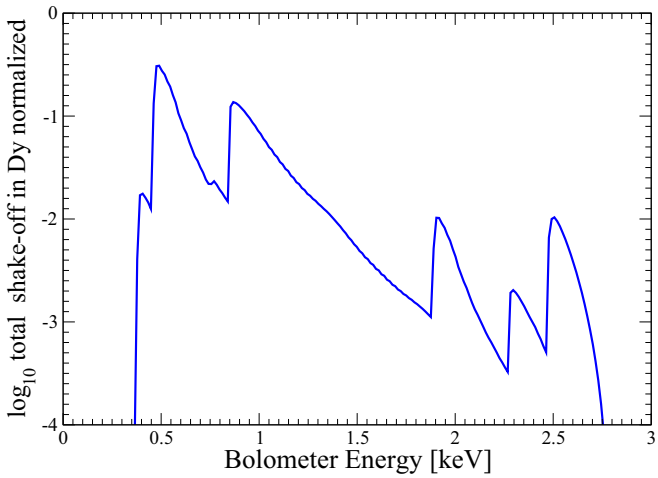

FIG. 10. Theoretical results of the sum of all s-waves shake-off contributions. The steep rise on the left of the maxima is connected with the binding energy of the two-hole states (see Table III), which contribute to the excitation of Dy. The rise is softened by the width of these states (Table III). The shake-off continuum contribution has to be added on top of these two-hole contributions. The energy difference between $Q = 2.8$ keV and E_c is carried away by the neutrino and does not show in the bolometer spectrum. The theoretical results are adjusted to the experiment [4,21] at the $N1,4s_{1/2}$ peak in Fig. 8.

V. CONCLUSIONS

In this work the effect of shake off on the de-excitation spectrum of the $^{163}_{66}$Dy* atom after electron capture in $^{163}_{67}$Ho for the determination of the electron neutrino mass is investigated. The electron neutrino mass is the difference between the Q value and the upper end of the de-excitation spectrum of Dy* measured by a bolometer. After capture the Dy* can be excited into one-hole and into two-hole electron configurations. The three-hole excitations and higher can be neglected [30]. The total two-hole excitation probability is given in the sudden plus the Vatai [7,8] approximation, not used here, by unity minus the overlap squared between Ho and Dy with the number of electrons in the exponent with the same quantum numbers in Dy as in Ho for the orbits, from which the particle is captured Eqs. (2) and (3):

$$(1.0 - \langle \mathrm{Ho},n,\ell,j|\mathrm{Dy},n,\ell,j\rangle^{(2(2j+1))}). \tag{24}$$

These Ho-Dy overlaps have in self-consistent relativistic Dirac-Hartree-Fock values of about 0.999 and even closer to unity (see Tables II and IV). Thus this total two-hole probability including also shake-off must be according to this rough estimate less than 0.4% of the one-hole excitation. This estimate is only very approximate. Important is the fact, that a small uncertainty of for example 10% for this overlap of the electron orbits in Ho and Dy produces a large increase of about two orders of magnitude for shake-off. Without using Vatai [7,8] the requirement for the norm (2) yields an upper limit for shake-off of 12% of the one-hole excitation and for a 10% error in the single electron overlaps between Ho and Dy no restriction at all (the upper limit for the shake-off probability is more than 100% relative to one-hole excitation). This means with 10% error the norm (2) would allow a shake-off probability larger than the one-hole excitation. The excited Dy* wave functions are calculated in a previous investigation [9,10] in first order with the perturbation (5) starting from Ho states based on pure Coulomb waves in Ho. A 10% error in the overlap produces an overestimation of shake-off by about two orders of magnitude. The bound states in Ho and Dy are described here in our work by the Dirac-Hartree-Fock approach [12–14] even including different occupations in Dy due to the hole states. The s-wave continuum wave functions in Dy are determined with the Dirac equation in the self-consistent potential [11]. The energy of the continuum states involved are limited by energy conservation to the Q value minus the two-hole binding energies, e.g., the $3s_{1/2}$, $4s_{1/2}$ two-hole state limits the upper bound of the continuum energy contributions to 2.8–2.4742 = 0.3258 keV. So this contribution is very small. One of the two main contributions comes from $4s_{1/2}$, $4s_{1/2}$ with a binding energy of 0.841 keV and thus an upper limit of the continuum energy of 2.8–0.841 = 1.959 keV. The second largest contribution is built on the two-hole state $4s_{1/2}$, $5s_{1/2}$ with the binding energy 0.4398 keV. Thus the upper limit of the shake-off contributions in the continuum integration (7) is the 2.8–0.4398 = 2.3602 for the integral over the shake-off continuum electron.

We prepared two different computer programs both calculating the s-wave shake-off to test the two codes against each other. All the calculations are done in double precision and

for the critical integrations we use parallel the Trapez, the Kepler-Simpson, the Bode, and the Weddle rules to test the accuracy. The numbers given are the ones from the Bode rule. (Trapez is not reliable enough.) The contributions from the shake-off process are small (see Figs. 7 and 8). The widths for the shake-off states include only the values from the two-hole excitations as in Ref. [9]. In reality one has to include the escape width of the electron in the continuum, which could perhaps even be larger than the contribution of the two-hole states.

In summary this work shows that one has not to worry about the shake-off process in the determination of the neutrino mass from electron capture in ^{163}Ho.

The remaining discrepancies between theory and experiment, e.g., the slope above the one-hole state $4s_{1/2}$ ($N1$), are probably due to configuration mixing not included here. Finally we want to stress, that the accuracy needed to extract the neutrino mass cannot be obtained by theoretical calculation alone. One must fit the neutrino mass, the Q value, the highest resonance hole energy, its width, and strength at the upper end of the spectrum to extremely accurate data.

ACKNOWLEDGMENTS

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