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Molecular effects in tritium β decay. IV. Effect of crystal excitations on neutrino mass determination

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We have computed the excitation probabilities of the T_2 molecules in the crystal surrounding the β-decaying tritium. The influence of this effect on the neutrino mass determination has been studied. For a neutrino mass of the order of a few eV the effect has been shown to be very important. Its importance decreases, however, with increasing neutrino mass. In addition we consider the influence of the high-energy portion ($E > 164$ eV) of the probability distribution on the neutrino mass.

I. INTRODUCTION

In a series of papers[1-5] we have presented theoretical results needed to interpret the measured β spectrum of T_2 and to extract information on the neutrino mass from this spectrum. The results are complete if T_2 is in the gas phase, as in Ref. 6. If, however, frozen T_2 is used, as in Ref. 7, additional problems arise due to the close proximity of nearby molecules. In Ref. 3, henceforth referred to as paper III, we have argued that most of the solid-state effects are small. We pointed out, however, two effects which might be non-negligible. The first one is due to multiple scattering of the emitted β electron on the other T_2 molecules in the solid. This effect can be experimentally determined by varying the source thickness. The second effect arises from possible molecular excitations in the solid caused by the sudden creation of a net positive charge due to the transformation of a neutral T_2 molecule into a HeT^+ molecular ion. This effect and its influence on the neutrino-mass determination is studied in the present work.

A perturbation-theory approach is used and the relevant formulas are derived in Sec. II. In Sec. III computations of the excitation probabilities are reported. In Sec. IV we show the results of our calculations. The importance of high excitations ($E > 164$ eV), neglected in our previous work,[3,4] is discussed in Sec. V.

II. THEORY

The total probability amplitude for a T_2 molecule undergoing a β decay in a crystal is given by an expression analogous to that used in paper III,

$$T_{if} = \langle \Phi^f \mid H_\beta \mid \Phi^i \rangle \ , \tag{1}$$

where now the initial and final functions for the whole system are defined as

$$\Phi^i = \chi^i_{\mathrm{nucl}} \psi^i_{\mathrm{T}_2} \prod_\alpha \psi^{i\alpha}_{\mathrm{T}_2} \ , \tag{2}$$

$$\Phi^f = \Omega^{-1/2} \chi^f_{\mathrm{nucl}} \exp(i \mathbf{k}_{\bar{\nu}} \cdot \mathbf{R}_{\bar{\nu}}) \psi^f_{\mathrm{HeT}} \prod_\alpha \psi^{f\alpha}_{\mathrm{T}_2} \ . \tag{3}$$

The notation above is consistent with that of paper III. $\psi^i_{\mathrm{T}_2}$ denotes the initial wave function of the active (decaying) T_2 molecule, while the wave functions $\psi^{i\alpha}_{\mathrm{T}_2}$ describe the inactive (spectator) molecules of the crystal. After the decay the active molecule transforms into the HeT^+ ion and the β electron. This system of two nuclei and three electrons is described by Ψ^f_{HeT}. In the initial state all the molecules are in their ground states. Since in the final state the active T_2 molecule changed into HeT^+, all the spectator T_2 molecules are now perturbed by the field of the ion. Some of them will also be excited by the time-dependent perturbation due to the sudden creation of the charged HeT^+ ion. All interactions between tritium molecules and any influence of the spectator molecules on the wave function of the HeT^+ ion are negligible and have been neglected. The experimental source thickness allowed us to assume infinite dimensions of the crystal.

Since H_β acts only on the coordinates of the decaying T_2 molecule, we immediately have

$$T_{if} = T'_{if} \prod_\alpha \langle \psi^{f\alpha}_{\mathrm{T}_2} \mid \psi^{i\alpha}_{\mathrm{T}_2} \rangle = T'_{if} \prod_\alpha T^\alpha_{if} \ , \tag{4}$$

where T'_{if} is the probability amplitude considered in paper III, i.e., that of the free decaying T_2 molecule. Since the effect of nuclear motion is small even in the active molecule,[3] we can safely neglect it in the spectator T_2 molecules, and we may write

$$T_{if}^{\alpha}=\langle \psi_n^{f\alpha} \mid \psi_0^{i\alpha} \rangle \ , \tag{5}$$

where $\psi_0^{i\alpha}$ is the ground-state electronic wave function for a T_2 molecule at equilibrium separation and $\psi_n^{f\alpha}$ are the wave functions of the final electronic states of the polarized spectator molecules. To simplify the notation we have suppressed the index T_2 in the wave functions and introduced instead an index specifying the electronic state of the molecule. Notice that due to the clamped-nuclei assumption there is now no distinction between T_2 and other isotopic species of the hydrogen molecule. We will, however, refer to the T_2 molecule for consistency.

Not only will the spectator T_2 molecules change their energies due to polarization interactions, one or more of them can also be excited from the ground state. The shift of the total energy of the crystal caused by the polarization of the spectator molecules by the net charge of the HeT^+ ion is independent of the final state of the latter and has no effect on the deduced neutrino mass; it only leads to an overall 0.88 eV shift of the β spectrum (paper III). The excitations of the polarized T_2 molecules, however, may be of some importance. To determine this effect we must solve the electronic Schrödinger equation for various excited states of a T_2 molecule in the external field,

$$H^{\alpha}\psi_n^{f\alpha}=E_n^{f\alpha}\psi_n^{f\alpha} \ , \tag{6}$$

where H^{α} contains the clamped-nuclei Hamiltonian H_0^{α} for the αth T_2 molecule plus the Coulombic interaction terms between the particles of HeT^+ and T_2. If not stated otherwise, atomic units will be used throughout this paper. Since the distance between T_2 and HeT^+ is large, we may replace the interaction part of the Hamiltonian by the interaction of T_2 with a positive charge located at the center of HeT^+,

$$H^{\alpha}=H_0^{\alpha}+\frac{1}{R_{T_1}^{\alpha}}+\frac{1}{R_{T_2}^{\alpha}}-\frac{1}{r_1^{\alpha}}-\frac{1}{r_2^{\alpha}}=H_0^{\alpha}+V^{\alpha} \ , \tag{7}$$

where $R_{T_i}^{\alpha}$ and r_j^{α} denote the distance from nucleus i and from electron j, respectively, to the charge.

Because the interaction with the charge is small, the above problem can be best solved by using first-order perturbation theory, i.e., by approximating the perturbed function of a T_2 molecule in its nth state by

$$\psi_n^{f\alpha}\cong c_{nn}^{\alpha}\psi_n^{i\alpha}+\psi_n^{\alpha(1)} \ , \tag{8}$$

where

$$\psi_n^{\alpha(1)}=\sum_{k(\neq n)} c_{nk}^{\alpha}\psi_k^{i\alpha} \ . \tag{9}$$

The coefficients c_{nk}^{α} are given by the familiar perturbation-theory expression

$$c_{nk}^{\alpha}=(E_n^i-E_k^i)^{-1}\langle \psi_k^{i\alpha} \mid V^{\alpha}\psi_n^{i\alpha}\rangle \quad \text{for } n\neq k \ . \tag{10}$$

Since the denominator in Eq. (10) is the same for all α, we do not use the index α for the energy of the unperturbed T_2 molecules. The initial wave functions on the αth center are assumed to form an orthonormal set and the final wave functions to be normalized to unity. Thus the coefficients c_{nk}^{α} fulfill the relation

$$\sum_k \mid c_{nk}^{\alpha} \mid^2=1 \ . \tag{11}$$

Upon substitution of the first-order wave function (8) into Eq. (5) for the probability amplitude we see immediately that the only contribution to T_{if} comes from

$$T_{if}^{\alpha}(n)\equiv\langle \psi_n^{f\alpha} \mid \psi_0^{i\alpha}\rangle=c_{n0}^{\alpha} \ . \tag{12}$$

The coefficient c_{00} [not defined by Eq. (10)] is obtained from Eq. (11). Since $c_{n0}^{\alpha}=-c_{0n}^{\alpha *}$, the sum of all $\mid T_{if}^{\alpha}(n)\mid^2$ is equal to 1 [cf. Eq. (11)].

In our calculations we further assumed that the interaction with the external charge in the Hamiltonian can be approximated by the first term of its multipole expansion. This approximation is justified by the large intermolecular distances in the T_2 crystal. Thus

$$V^{\alpha}=(\mathbf{r}_1+\mathbf{r}_2)\cdot\hat{\mathbf{n}}_{\alpha}R_{\alpha}^{-2} \ , \tag{13}$$

where $\mathbf{r}_i$ is the radius vector of the ith electron of the T_2 molecule under consideration, and $\hat{\mathbf{n}}_{\alpha}$ is the unit vector pointing from the center of the αth molecule towards the external charge.

Using the potential given by Eq. (13) we can write

$$\mid c_{n0}^{\alpha}\mid^2=a_n^{\alpha}R_{\alpha}^{-4} \ , \tag{14}$$

where for $n\neq 0$,

$$a_n^{\alpha}=\mid \langle \psi_0^{i\alpha} \mid (\mathbf{r}_1+\mathbf{r}_2)\cdot\hat{\mathbf{n}}_{\alpha} \mid \psi_n^{i\alpha}\rangle \mid^2/(E_0^i-E_n^i)^2 \ , \tag{15}$$

and R_{α} denotes the distance of the αth molecule from the charge.

Obviously $\mid c_{n0}^{\alpha}\mid^2$ represents the probability of exciting the αth molecule to the state n. One can also introduce the transition probability for the molecule α to be excited to any state,

$$\sum_{n(\neq 0)} \mid c_{n0}^{\alpha}\mid^2=R_{\alpha}^{-4}\sum_{n(\neq 0)} a_n^{\alpha}\equiv R_{\alpha}^{-4}a^{\alpha} \ . \tag{16}$$

Due to the small anisotropy of T_2 and a fairly free rotation of the molecules in the crystal we may neglect the explicit orientations of the molecules and average over the directions of $\hat{\mathbf{n}}_{\alpha}$. This average gives

$$a_n=\langle a_n^{\alpha}\rangle=\tfrac{1}{3}(X_{0n}^2+Y_{0n}^2+Z_{0n}^2) \ , \tag{17}$$

where

$$X_{0n}=(E_n^i-E_0^i)^{-1}\langle \psi_0^i \mid x_1+x_2 \mid \psi_n^i\rangle \ , \tag{18}$$

and similarly for Y_{0n} and Z_{0n}. In Eq. (17) we assumed that the transition moments X_{0n}, Y_{0n}, and Z_{0n} are real. Since the choice of the coordinate system for each molecule is now arbitrary, we have chosen the z axis to coincide with the molecular axis. We have also suppressed the index α in the unperturbed wave function because for the body-fixed coordinate system the transition moments are independent of α. Similarly we introduce the constant a obtained by averaging a^{α} over orientations or summing a_n over n.

The energy of the perturbed T_2 molecule is given by

$$E_n^{f\alpha}=E_n^i+E_n^{\alpha(2)}=E_n^i+\sum_{k(\neq n)}|c_{nk}^{\alpha}|^2(E_n^i-E_k^i)\ . \tag{19}$$

With the approximation to Eq. (13) the first-order energy vanishes due to symmetry reasons. If the exact V^{α} of Eq. (7) were used, the first-order correction would appear in Eq. (19). This correction would, however, become zero after averaging over T_2 orientations.

When $E_n^{f\alpha}$ is averaged over orientations of the T_2 molecules, we find that $\bar{E}_n^{f\alpha}=E_n^i-\frac{1}{2}\bar{\alpha}_n R_{\alpha}^{-4}$, where $\bar{\alpha}_n$ is the isotropic polarizability of the nth electronic excited state of T_2. Assuming that only one spectator T_2 molecule can be excited (it will be shown later that double excitations appear with negligible probabilities), the energy E of the final state of the crystal is given by

$$E_{jn}=E_j^f+E_n^i-\tfrac{1}{2}\bar{\alpha}_0\sum_{\gamma}R_{\gamma}^{-4}+\tfrac{1}{2}(\bar{\alpha}_0-\bar{\alpha}_n)R_{\alpha}^{-4}\ , \tag{20}$$

where j and n specify the excited states of the HeT^+ ion and T_2 molecule, respectively, and R_{α} denotes the distance between the excited T_2 molecule and the HeT^+ ion. **The third term on the right-hand side of Eq. (20) was estimated in paper III to be equal to -0.88 eV. This term shifts only the energy scale and has no influence on the neutrino-mass determination. The last term on the rhs of Eq. (20) does depend on the final state of the crystal but it can be neglected since it is much smaller than the excitation energies E_n^i. Thus our final energies are approximated as $E_{jn}=E_j^f+E_n^i$ (or $E=E_j^f+E_{n_1}^i+E_{n_2}^i+\cdots$, if multiple excitations are also considered).**

Now we can easily calculate the probability distribution. The probability corresponding to the amplitude given by Eqs. (1) or (4) can be expressed as

$$P_{if}=|T_{if}|^2\equiv P(j,n_1,n_2,\ldots)=P'(j)\prod_{\alpha}P^{\alpha}(n_{\alpha})\ , \tag{21}$$

where j labels the final states of the HeT^+ ion and n_{α} the final states of the αth spectator molecule. The probabilities $P'(j)$ are given in Ref. 4 and $P^{\alpha}(n)$ are obtained by averaging $|T_{if}^{\alpha}(n)|^2=|c_{0n}^{\alpha}|^2$ over molecular orientations,

$$P^{\alpha}(n)=\begin{cases}1-aR_{\alpha}^{-4} & \text{for } n=0\ ,\\ a_nR_{\alpha}^{-4} & \text{for } n\neq 0\ .\end{cases} \tag{22}$$

To connect the probability (21) with experiment it is convenient to use the quasicontinuous parameter E rather than j and n. Thus we can write

$$P_{if}=P(j,n_1,n_2,\ldots)\equiv P(E)\ , \tag{23}$$

where

$$E=E_j^f+E_{n_1}^i+E_{n_2}^i+\cdots\ .$$

It should be recalled that all T_2 molecules are initially in their ground states. This lowest energy will be taken as the reference value, and therefore E represents the excitation energy of the whole system.

By performing a summation over all final states of the crystal corresponding to the total energy E, one gets the probability distribution

$$P(E)=P'(E)P_{0+}\sum_{n(>0)}P'(E-E_n^i)P_n+\sum_{\substack{n,m\\(0<n<m)}}P'(E-E_n^i-E_m^i)P_{nm}+\cdots\ , \tag{24}$$

where P_0 is the probability that no T_2 molecule is excited, P_n is the probability that only one T_2 molecule is excited to the energy E_n^i, P_{nm} is the probability that two molecules are excited to the energy $E_n^i+E_m^i$, etc., and $P'(E)$ is the probability distribution listed in Table I of Ref. 4.

Using Eqs. (21) and (22) we easily find that

$$P_0=\prod_{\alpha}(1-aR_{\alpha}^{-4})\simeq 1-a\sum_{\alpha}R_{\alpha}^{-4}=1-afd^{-4}\ , \tag{25}$$

In Eq. (25) we used the fact that $\sum R_{\alpha}^{-4}=fd^{-4}$, where d denotes the nearest-neighbor distance in the crystal lattice and $f=25.3383$ (see Ref. 8). Similarly, for P_n and P_{nm} we obtain

$$P_n=\sum_{\alpha}P^{\alpha}(n)\prod_{\gamma(\neq\alpha)}P^{\gamma}(0)=fa_nd^{-4}\ , \tag{26}$$

$$P_{nm}=\sum_{\substack{\alpha,\beta\\(\alpha\neq\beta)}}P^{\alpha}(n)P^{\beta}(m)\prod_{\gamma(\neq\alpha,\beta)}P^{\gamma}(0)\simeq f^2a_na_md^{-8}\ . \tag{27}$$

Due to the small value of the fa_nd^{-4} factors (see Secs. III and IV) we neglect terms of the order of d^{-8} in Eq. (26), and the probabilities of all multiple excitations, as given, e.g., by Eq. (27).

III. TRANSITION MOMENTS

To evaluate the probability distribution (24), we need transition moments given by Eq. (18) and the corresponding energies of the excited states. From the symmetry it follows immediately that $z_{0n}\neq 0$ only if n denotes a ${}^1\Sigma_u^+$ state, whereas x_{0n} $(=y_{0n})\neq 0$ only if n denotes a ${}^1\Pi_u^+$ state. The three lowest ${}^1\Sigma_u^+$ states are usually denoted as B, B', and B'' in spectroscopy; for the lowest ${}^1\Pi_u^+$ states the notation C, D, D', and D'' is used.

As in our previous work (Refs. 1, 3, and 5) all wave functions for the singlet states under consideration were assumed in the form of expansions

$$\Psi=\sum_j C_j[\Phi_j(\mathbf{r}_1,\mathbf{r}_2)x_1^l+(-1)^{s_j+\bar{s}_j+k}\Phi_j(\mathbf{r}_2,\mathbf{r}_1)x_2^l]\ , \tag{28}$$

with the basis functions defined by

$$\Phi_j(\mathbf{r}_1,\mathbf{r}_2)=\exp(-\alpha\xi_1-\bar{\alpha}\xi_2-\beta\eta_1-\bar{\beta}\eta_2)\xi_1^{r_j}\xi_2^{\bar{r}_j}\eta_1^{s_j}\eta_2^{\bar{s}_j}\rho^{\mu_j}\ , \tag{29}$$

where ξ and η denote the elliptic coordinates; $\rho = 2r_{12}/R$; r_{12} and R denote the interelectronic and internuclear distances, respectively; α, $\bar{\alpha}$, β, and $\bar{\beta}$, as well as c_j in Eq. (28), are variational parameters; r_j, $\bar{r}_j$, s_j, $\bar{s}_j$, and μ_j are integers; $k=0$ for Σ_g and Π_u states; $k=1$ for Σ_u and Π_g states; and $l=0$ or 1 for Σ and Π states, respectively. For the ground state we used a 69-term wave function obtained from the 80-term expansion[9] by neglecting terms with the third powers of the interelectronic distance. In this wave function we optimized all four nonlinear parameters, thus getting $E=-1.174\,473\,6$, only 1.1 μhartree higher than the most accurate value.[10] For the B, B', and B'' states we used the 88-, 80-, and 76-term expansions,[11,2] respectively. In the previous work[11,12] the exponents for these states had not been optimized in the above full expansions but rather in some shorter ones. Since this might affect the accuracy of the transition probabilities, we reoptimized the nonlinear parameters using the full expansions.

The results of our calculations are shown in Table I. For both the energy E and the transition moment $z_{0n} = Z_{0n}(E_n^i - E_0^i)$, the upper entry corresponds to the literature wave functions as described above, whereas the lower one has been obtained using wave functions with exponents optimized in the present work. The change in transition moments is seen to be insignificant. The value of z_{0n} for the B state is in agreement with the recent result of Dressler and Wolniewicz[13] who obtained $z_{0B} = 0.9821$ with somewhat different wave functions. The small difference between their and our value may be due to a more accurate ground-state wave function used in their work. We may also point out that our new energies listed as lower entries in Table I are the best known values for these states. They indicate that by improving the clamped-nuclei potential-energy curves one can decrease the still existing discrepancy between theoretical and experimental term values.[14]

For the B'' state we found that the energy given for the internuclear distance $R=1.4$ bohr in Ref. 12 represents the fourth eigenvalue rather than the third one. In that work the complete diagonalization of the Hamiltonian matrix was not performed, and only a single eigenvalue was computed, located in an assumed region of energy. It happened that for $R=1.4$ bohr the computation[12] converged to the four eigenvalue. Hence for this state also the upper entry in Table I differs slightly from the published value.[12] We checked, however, that for larger internuclear distances the B''-state energies published in Ref. 12 correctly represent the third eigenvalue, though they are certainly improvable. Thus, e.g., for the equilibrium internuclear distance $R=2.025$ bohr, by only optimizing the exponents in the 76-term expansion we lowered the energy by 50 μhartree ($=11$ cm^{-1}).

TABLE I. Energies and transition moments, $z_{0n} = Z_{0n}(E_n^i - E_0^i)$ (and similarly for the x component), for the three lowest $^1\Sigma_u^+$ and $^1\Pi_u^+$ states of the hydrogen molecule at $R=1.4$ bohr (all quantities in atomic units).

State	E_n	z_{0n}	x_{0n}
B	$-0.705\,772\,68$[a]	0.9813	
	$-0.705\,774\,71$	0.9814	
B'	$-0.628\,662\,95$[b]	0.3979	
	$-0.628\,673\,05$	0.3980	
B''	$-0.602\,492\,58$[b]	0.2305	
	$-0.602\,543\,32$	0.2345	
C	$-0.688\,662\,35$		0.7433
D	$-0.623\,525\,15$[c]		0.3389
	$-0.623\,545\,92$		0.3395
D'	$-0.601\,106\,13$		0.0018

[a] Reference 11.

[b] Reference 12.

[c] Reference 15.

Using the optimized exponents and the 88-, 80-, and 76-term expansions determined for the three $^1\Sigma_u^+$ states, respectively, we computed and diagonalized the Hamiltonian matrices. This gave us three sets of eigenvalues, denoted I, II, and III, and the corresponding eigenvectors which were used to compute the transition moments. These transition moments are for the molecular axis parallel to the direction of the electric field. The computed energies and the values of Z_{0n}^2, which divided by R_α^4 give the transition probabilities, are listed in Table II. For brevity, we give results only for those values of n for which $Z_{0n}^2 > 0.0005$. It is seen that for all three expansions the total probabilities of excitations are not much different. However, their distributions, as functions of excitation energy, differ considerably. The B''-state wave function has the smallest exponents for one of the electrons. Therefore, one may expect that this expansion is best suited to describe not only this particular state but also the higher singly excited Rydberg-type states. Consequently, it seems that from the available data the most reliable description of excitations is given by column III in Table II, provided the first two entries are replaced by the more accurate values for the B and B' states, from columns I and II, respectively. This gives $\sum Z_{0n}^2 = 6.1039$.

A similar procedure has been employed to compute the transition moments for the $^1\Pi_u^+$ states. For the C and D states we have used the 80-term expansions selected previously.[15] For the D' state the same expansion has been used as for the D state. For each of the three states the exponents have been independently optimized resulting in some improvement over the best previous energies. The computed energies and the transition moments are listed in Table I. These transition moments are for the molecular axis perpendicular to the direction of the electric field. For the C state our result is very close to the value obtained recently by Dressler and Wolniewicz,[13] $x_{0n} = 0.7432$, using somewhat different wave functions.

In Table III we list the energies and the values of X_{0n}^2 $(=Y_{0n}^2)$ computed using three different expansions for the $^1\Pi_u^+$ state. The columns denoted I, II and III correspond to 80-term wave functions with exponents optimized for the first, second, and third eigenvalue, respectively. Although the probability distributions among various states differ considerably for the three expansions, the total probability of transitions to all $^1\Pi_u^+$ states is much less sensitive to the expansion used. Some spe-

TABLE II. Energies and probabilities of excitations (multiplied by R_α^4) to the $^1\Sigma_u^+$ states of the hydrogen molecule, at $R=1.4$ bohr, computed using wave functions with exponents optimized for the B (I), B' (II), and B'' (III) states, respectively; only states with $Z_{0n}^2>0.0005$ are included (all quantities in atomic units).

	I			II			III	
n	E_n	Z_{0n}^2	n	E_n	Z_{0n}^2	n	E_n	Z_{0n}^2
1	−0.705 774 71	4.3844	1	−0.705 748 45	4.3805	1	−0.705 346 84	4.2783
2	−0.626 366 56	0.6476	2	−0.628 673 05	0.5318	2	−0.628 530 35	0.5157
3	−0.563 863 99	0.6366	3	−0.602 120 55	0.1851	3	−0.602 543 32	0.1681
4	−0.561 993 72	0.0077	5	−0.579 285 43	0.2761	5	−0.576 848 90	0.3783
5	−0.386 360 85	0.4361	6	−0.508 601 60	0.5900	7	−0.373 742 23	0.6316
6	−0.374 589 06	0.0028	8	−0.142 396 92	0.1492	8	−0.019 667 47	0.0016
7	−0.043 150 48	0.0057	9	−0.017 884 90	0.0065	9	0.067 313 10	0.0007
8	0.057 032 17	0.0097	10	0.052 413 20	0.0009	10	0.072 695 78	0.0008
9	0.106 833 81	0.0032	12	0.145 585 24	0.0008	11	0.103 940 90	0.0014
10	0.125 766 98	0.0126	15	0.245 595 23	0.0005	22	0.643 816 27	0.0011
11	0.216 009 69	0.0012	25	0.670 239 72	0.0011	23	0.705 420 83	0.0006
						25	0.788 460 02	0.0009
Remaining states		0.0014			0.0024			0.0026
$\sum Z_{0n}^2$		6.1490			6.1249			5.9817

cial features of the probability distribution are also reproduced in all three expansions. For example, the probability of transition to the third state is practically zero in all three cases. Similarly, as for the $^1\Sigma_u^+$ states, it seems that the probabilities listed in column III, with the first two entries replaced by those from columns I and II, respectively, would represent a judicious choice for describing transitions to the $^1\Pi_u^+$ states. This gives $\sum X_{0n}^2=3.9314$.

IV. EFFECT ON NEUTRINO-MASS DETERMINATION

To study the effect of crystal excitations on the neutrino-mass determination a new probability distribution was obtained according to Eqs. (24)–(26). First, the 155 probabilities P'_{if} from Table I of Ref. 4 were multiplied by the probability of nonexcitation P_0 given by Eq. (24). The total excitation probability was obtained from

TABLE III. Energies and probabilities of excitations (multiplied by R_α^4) to the $^1\Pi_u^+$ states of the hydrogen molecule, at $R=1.4$ bohr, computed using wave functions with exponents optimized for the C (I), D (II), and D' (III) states, respectively; for $n>3$ only states with $X_{0n}^2>0.0005$ are included (all quantities in atomic units).

	I			II			III	
n	E_n	X_{0n}^2	n	E_n	X_{0n}^2	n	E_n	X_{0n}^2
1	−0.688 662 35	2.3408	1	−0.688 572 05	2.3287	1	−0.687 908 55	2.2441
2	−0.620 750 56	0.4939	2	−0.623 545 92	0.3798	2	−0.623 319 52	0.3674
3	−0.581 051 04	0.0000	3	−0.599 474 39	0.0004	3	−0.601 106 13	0.0000
4	−0.559 380 77	0.5437	4	−0.598 866 62	0.1823	4	−0.600 276 24	0.1290
5	−0.447 086 69	0.0010	5	−0.567 187 44	0.3043	5	−0.588 371 95	0.0847
6	−0.425 129 24	0.4405	6	−0.564 610 28	0.0014	7	−0.571 205 96	0.2162
7	−0.104 453 26	0.1734	7	−0.486 550 78	0.5197	9	−0.464 852 08	0.7760
10	0.122 863 79	0.0007	9	−0.111 260 80	0.2617			
19	0.494 944 87	0.0017						
23	0.742 115 07	0.0012						
25	0.777 115 61	0.0019						
26	0.835 064 80	0.0016						
28	0.931 057 35	0.0022						
33	1.128 766 45	0.0009						
34	1.175 661 38	0.0007						
35	1.261 051 17	0.0008						
Remaining states		0.0024			0.0022			0.0048
$\sum X_{0n}^2$		4.0074			3.9805			3.8222

the values listed in columns III of Tables II and III, replacing the first two entries with those from columns I and II, respectively. Using for the nearest-neighbor distance in T_2 the value (see paper III) $d = 6.68$ bohr, we obtained $P_0 = 0.940\,757$.

To compute the probabilities of single excitations, we applied in Eq. (26) the values $a_n = Z_{0n}^2/3$ for the ${}^1\Sigma_u^+$ states from Table II and the values $a_n = 2X_{0n}^2/3$ for the ${}^1\Pi_u^+$ from Table III. Only eight states with $Z_{0n}^2 > 0.001$ were taken into account. For the B and B' states we have used the values from columns I and II of Table II, respectively. For the B'' state and the five higher ${}^1\Sigma_u^+$ states we employed the values from column III of the same table. For the C and D states we have used the results from columns I and II of Table III, respectively. For the D' state the probability is zero, and for the four higher ${}^1\Pi_u^+$ states we have used the probabilities from column III of Table III. Thus, in total, eight ${}^1\Sigma_u^+$ and six ${}^1\Pi_u^+$ states were considered. The energies and probabilities for these states are given in Table IV. The 155 probabilities from Table I of Ref. 4 were multiplied consecutively by each of the 14 probabilities and, in accordance with Eq. (23), the corresponding energies were shifted by the excitation energies of T_2.

The resulting probability distribution $P(E)$, given by Eq. (24), was thus composed of 155 values of $P'(E_j)P_0$ and of 2170 values of $P'(E_j)P_n$. Probabilities smaller than 10^{-5} were rejected and the remaining 1580 values were used in the computation performed similarly as in paper III. The new probability distribution was used to construct the reference spectrum for various assumed neutrino masses and the spectrum determined by the probability distribution of Ref. 4 was fitted to it. The spectra have been convoluted with a Gaussian resolution function of 4.7 eV width. No statistical deviations have been added to the reference spectrum since we have checked in paper III that this procedure has practically no effect on the final conclusions, and it consumes substantially more computer time due to the necessity of performing a large number of fits with different sets of random numbers. The fits were made in a 400-eV range beginning from 50 eV above the endpoint. The integration step was 0.1 eV. The reference endpoint energy for zero neutrino mass W_0 was 18 580 eV as in paper III.

The results of our computations are listed in Table V, where $m_{\bar{\nu}}$ and $\tilde{m}_{\bar{\nu}}$ denote the neutrino mass used in the reference spectrum and in the fitted one, respectively. It is seen that for a large neutrino mass (30 eV) the effect of crystal excitations, although not negligible, is not very significant. It becomes, however, progressively more important for smaller neutrino masses.

TABLE IV. Probabilities P_n of Eq. (26) used in the calculation of the β-decay spectrum. The ground-state energy of T_2 is assumed to be $E_0 = -1.174\,475\,677$ a.u.

n	Symmetry	$E - E_n^i$ (eV)	P_n
1	Σ	12.754 05	0.018 598
2	Π	13.219 70	0.019 858
3	Σ	14.852 11	0.002 256
4	Π	14.991 62	0.003 222
5	Σ	15.563 14	0.000 713
6	Π	15.624 83	0.001 094
7	Π	15.948 76	0.000 719
8	Σ	16.262 32	0.001 605
9	Π	16.415 88	0.001 834
10	Π	19.309 94	0.006 583
11	Σ	21.789 18	0.002 679
12	Σ	31.424 12	0.000 007
13	Σ	34.787 70	0.000 006
14	Σ	49.478 58	0.000 005

To check the sensitivity of the results to the accuracy of the probability distribution we rejected 528 probabilities that were smaller than 10^{-4}, and used the remaining 1046 values to determine the neutrino mass. This had practically no effect on the result, changing $\tilde{m}_{\bar{\nu}}$ by only 0.03 eV for $m_{\bar{\nu}} = 4.0$ eV. The negligible effect of the small probabilities also shows that the double excitations, due to the factor $f^2/d^8 = 0.000\,16$ [cf. Eq. (27)], could be safely neglected.

V. EFFECT OF TRANSITIONS TO HIGHLY EXCITED CONTINUUM STATES

Another problem connected with the accuracy of the neutrino-mass determination using the probability distribution given in Ref. 4 results from truncating the probability distribution. These probabilities are listed for excitation energies smaller than 164.173 eV. They correspond to the lowest 100 eigenvalues obtained in computations involving 200-term expansions, accounting for 99.489% of probability. The remaining 100 eigenvalues, accounting for 0.511% of probability, are spread over the next 600 eV. How accurate is a neutrino-mass determination performed without the high-energy transitions occurring with a total probability of 0.511%? To answer this question we have performed our fits with spectra modified to include 100% of probability.

From the 200-term computation performed at the equilibrium internuclear distance $R = 1.4$ bohr we took the 100 highest eigenvalues and the corresponding probabilities. These are distributed in the region between 167.8 and 759.3 eV, and account for 0.333% of probability. To obtain the remaining probability of 0.178% an averaging over the nuclear motion would have to be performed. We included this effect in the simplest possible way, namely, by multiplying the probabilities by a factor 0.511/0.333. These "renormalized" values were added to

TABLE V. Influence of crystal excitation on the neutrino-mass determination; $m_{\bar{\nu}}$ is the reference mass while $\tilde{m}_{\bar{\nu}}$ is the mass obtained with the neglect of the crystal excitations.

$m_{\bar{\nu}}$	3.25	3.4	3.5	4.0	5.0	7.0	30.0
$\tilde{m}_{\bar{\nu}}$	0.000	0.33	0.86	2.02	3.47	5.81	29.08

TABLE VI. Influence of the high-energy tail of the excitation spectrum of HeT^+ on the neutrino-mass determination; $m_{\bar{\nu}}$ is the reference mass while $\tilde{m}_{\bar{\nu}}$ denotes the mass obtained neglecting the probabilities for $E > 164$ eV.

$m_{\bar{\nu}}$	1	2	3	5	10
$\tilde{m}_{\bar{\nu}}$	0.00	1.68	2.78	4.86	9.90

the P'_{if} probabilities of Ref. 4 resulting in a probability distribution $\tilde{P}_{if}$ that is distributed in the region $0 < E < 759.3$ eV and which sums up to 100.000%.

To check the importance of the high-energy tail of the $\tilde{P}_{if}$ probability we took it as the reference probability distribution and proceeded in the usual manner. For an assumed neutrino mass $m_{\bar{\nu}}$ a reference spectrum was computed and the spectrum obtained from the truncated probability distribution P'_{if} was fitted to it. The best fit yielded the neutrino mass $\tilde{m}_{\bar{\nu}}$. The results are shown in Table VI. It is seen that for small neutrino masses the high-energy tail of the probability distribution is not negligible.

We also tested the applicability of some approximate probability representations to account for the "missing" 0.511%. These representations have been used to construct spectra that have been fitted to the reference spectrum obtained with the $\tilde{P}_{if}$ probability distribution. Since the sensitivity of the neutrino mass to this effect is significant only for small $m_{\bar{\nu}}$, we performed these tests only for $m_{\bar{\nu}} = 1$ eV.

When 0.511% was simply added to the last probability (0.002) at 164.173 eV in P'_{if}, we obtained $\tilde{m}_{\bar{\nu}} = 1.55$ eV, which shows that not only the incompleteness of the probability but also its distribution in the high-energy region is of importance for this small neutrino mass. Next we approximated the probability distribution for an excitation energy $E > E_0$ with the formula obtained using the asymptotic behavior of probabilities for the hydrogen atom (cf. Ref. 16),

$$P(E) = 2.5R(E_t)E_t^{5/2}E^{-7/2} , \qquad (30)$$

where $R(E_t)$ is the residual probability for $E \geq E_t$. If $E_t = 164.173$ eV, then $R(E_t) = 0.513\%$ (see Ref. 4).

If the spectrum obtained with the above probability distribution is fitted to the reference spectrum corresponding to $\tilde{P}_{if}$ and $m_{\bar{\nu}} = 1$ eV, one gets $\tilde{m}_{\bar{\nu}} = 1.02$ eV. Hence we are convinced that Eq. (30) satisfactorily represents the probability distribution at high energies.

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