Final-state spectrum of ^{3}He after β^- decay of tritium anions T^-

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The final-state spectrum of β decaying tritium anions T^- was calculated. The wave functions describing the initial T^- ground state and the final ^{3}He states were obtained by the full configuration-interaction method. The transition probability was calculated within the sudden approximation. The transition probability into the electronic continuum was extracted from the complex-scaled resolvent and shown to converge for very high energies to an approximate analytical model probability distribution.

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I. INTRODUCTION

The neutrino rest mass is a very important parameter for cosmology, astrophysics, and the standard model of elementary particles. The existence of neutrinos, already postulated by Pauli and put into a mathematical framework of β decay by Fermi [1] a long time ago, was verified by Reines and Cowan in 1956 [2]. However, despite the high solar neutrino flux of about billions per $m^{-2}\,s^{-1}$ on earth, the answer to the question about their rest mass is one of the big unknowns in physics. Because neutrino-flavor oscillations were observed in the late 1990s at the Super-Kamiokande experiment [3], a nonvanishing neutrino rest mass has to be expected. Unfortunately, this type of experiment reveals only mass differences between neutrino flavors.

The presently constructed KATRIN (Karlsruhe tritium neutrino mass) experiment with an expected sensitivity of about 0.2 eV (90% C.L.) should have the ability to determine the absolute value for one of the flavors or at least a new upper limit to it [4]. This so-called next-generation tritium β-decay experiment is only based on kinematic relations and energy and momentum conservation. Thus KATRIN provides a model-independent direct measurement of the antineutrino rest mass $m_{\bar{\nu}_e}$ (more accurately the mass of the antineutrino in a given mass-flavor mixture mostly attributed to the electronic neutrino). In more detail, $m^2_{\bar{\nu}_e}$ will be extracted in a fit procedure from the shape of the β spectrum. Besides the precise measurement of the β-electron energy spectrum, it is crucial for the mass extraction to know how the β spectrum is modified by the final-state spectrum of the decay product. As in the previous most recent tritium neutrino-mass experiments in Mainz and Troitsk, the T_2 molecule is chosen as the tritium source. T_2 comprises a compromise between experimental accessibility and theoretical treatability. The final-state spectrum of its decay product $^3HeT^+$ was therefore the subject of a number of very detailed calculations [5–14], finally accumulating in the one covering the whole energy regime [15]. Recently, the spectrum was further adapted to specific needs (isotope distribution and temperature) of the KATRIN experiment [16].

Although a high purity of the molecular tritium source is expected for KATRIN, the produced β electrons can interact with other gas molecules and thus produce tritium species different from T_2. One of the expected processes is the dissociative attachment,

$$e^- + T_2 \rightarrow T^- + T, \tag{1}$$

where T^- formation occurs. Despite the relative small cross section compared to, e. g., the one for vibrational excitation of the T_2 molecule, this process is very important. The reason is the higher end-point energy of the β spectrum for the decay of T^- compared to that of T_2. Due to this fact, the occurrence of T^- ions leads to a systematical error and hence to a possible limitation of the sensitivity of KATRIN, if it is not properly accounted for [17].

To the best of our knowledge, there exist so far only two theoretical predictions for the final-state spectrum following β decay of T^-. However, in [18] only transition probabilities to four final states are reported. Furthermore, the results in [18] disagree substantially from the ones given in an earlier work [19], which was, however, also limited to 10 final states. The aim of this work is thus to provide a complete final-state spectrum for the decay process

$$T^- \rightarrow {}^3\mathrm{He} + e^- + \bar{\nu}_e\,, \tag{2}$$

and to shed some light on the disagreeing earlier results.

II. METHOD AND COMPUTATIONAL DETAILS

The calculation of the nonrelativistic eigenstates of atomic systems is performed within the approximation of an infinitely heavy mass of the nuclei, i. e., $T \approx {}^\infty\mathrm{H}$ and $^3\mathrm{He} \approx {}^\infty\mathrm{He}$. This is justifiable because of the large mass difference of the nucleus and the electrons. The calculation of the final-state spectrum can be performed analytically for *neutral* T atoms and reveals a negligible mass dependence. Hence a large mass dependence is also not expected in the case of tritium anions. The nonrelativistic Hamiltonian for the two-electron system has the form (atomic units with $m_e = 1, e = 1, \hbar = 1$ are used throughout, if not specified otherwise)

$$\hat{H} = -\frac{1}{2}(\Delta_1 + \Delta_2) - Z\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \tag{3}$$

where Z is the charge of the nucleus and $\mathbf{r}_i$ the position vector of the ith electron. Because the only bound state of T^- is a singlet state with angular momentum $L = M = 0$ [20], only symmetric spatial configuration state functions (CSFs)

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are important, that is,

$$|\Phi_k^{(+)}\rangle = \begin{cases} 2^{-1/2}\left(|\phi_i\rangle|\phi_j\rangle + |\phi_j\rangle|\phi_i\rangle\right) & i \neq j, \\ |\phi_i\rangle|\phi_j\rangle & i = j. \end{cases} \tag{4}$$

To determine the eigenstates and corresponding energy eigenvalues, a simple expansion in Slater-type orbitals (STOs) is used,

$$\langle \mathbf{r}|\phi_i\rangle = \sqrt{\frac{(2\zeta_i)^{2n+1}}{(2n)!}}\, \exp(-\zeta_i r) r^{n-1}\, Y_l^m(\vartheta, \varphi). \tag{5}$$

The n, l, m are integer parameters with limitations analogous to the ones for the hydrogen quantum numbers, and the Y_l^m represent the spherical harmonics. The ζ_i are positive real parameters. An appropriate choice of these parameters allows the achievement of an, in principle, complete coverage of the Hilbert space of the one-particle part of Hamiltonian (3). In the full configuration-interaction (CI) method, the eigenstates are expressed as a linear superposition of all possible symmetry-adapted CSFs

$$|\Psi_j(\mathbf{r}_1, \mathbf{r}_2)\rangle = \sum_k c_{jk} |\Phi_k^{(+)}\rangle \tag{6}$$

that can be formed with the aid of the chosen STO basis. The expansion coefficients c_{jk} are determined by solving the generalized eigenvalue problem obtained from inserting the wave-function *ansatz* of Eq. (6) into the eigenvalue equation of the Hamiltonian (3).

The final-state spectrum of He is calculated within the sudden approximation [21] that is based on the fact that the escaping β electron has a much higher velocity than the bound electrons. In the analysis of tritium neutrino-mass experiments like KATRIN, only the β electrons with an energy near the end point of the β spectrum at 18.6 keV are used. Their velocity is clearly much larger than the average speed of the bound electrons in T^-. In fact, the validity of the sudden approximation has been demonstrated for T_2 in [10,12,22], where the first-order correction terms were derived and explicitly calculated. From those results, it is apparent that also for T^- the sudden approximation is expected to be valid within the accuracy required for the analysis of an experiment like KATRIN. Nevertheless, a brief discussion of possible effects beyond the sudden approximation on the final-state spectrum is given at the end of this work.

A basis set of 555 STOs yielding 3481 CSFs in the full CI calculation was used to obtain the final results shown in this work. This STO basis set contains all possible kinds of orbitals (with restrictions on l and m as mentioned above) up to the angular quantum number $l = 7$, $-7 \leqslant m \leqslant 7$. For the optimization of the parameters ζ_i, a genetic and several other algorithms [23] were tested. However, none of those algorithms led to completely convincing results. Therefore, the parameters were finally optimized by hand. The difficulty of the parameter optimization is caused by the requirement to construct a basis set with high coverage of the Hilbert space while avoiding inaccuracies due to numerically caused linear dependencies. With the aim to achieve a uniform description of the possible He final states, it is favorable to obtain a homogeneous and a high density of states in the continuum as well as a large number of bound states. If a large number of CFSs is used, the optimization of the individual ζ_i values becomes less important, since the full CI method leads to a sufficient mixing of the Hilbert space covered by the various STOs. Therefore, the parameters ζ_i were chosen to start in an interval between 2 and 3 and to decrease in value for increasing n (for a given l). This procedure avoids numerical problems and allows the construction of a huge, but linearly independent, basis set. This basis set is used for both the ground state of T^- and all final states of He. The chosen basis leads for T^- to the ground-state energy $E_0^{T^-} = -14.3602$ eV, which is only 0.8 meV above the very accurate values in [24,25]. In the case of He, the adopted basis set yields 16 states below the ionization continuum. Of those 16 states, 15 are identified as true physical states, while the 16th state is a pseudostate that resembles the remaining infinite number of Rydberg states; this is a consequence of the finiteness of the adopted basis set.

Within the sudden approximation, the transition probability for T^- decays into bound states of He is simply given by the squared overlap

$$P_n = \left|\langle \Psi_n^{He} | \Psi_i^{T^-} \rangle\right|^2 \tag{7}$$

of the initial state $|\Psi_i^{T^-}\rangle$, i. e., the T^- ground state, and the final state $|\Psi_n^{He}\rangle$, i. e., the nth bound state of He.

To calculate the transition-probability density into continuum states, the complex scaling method is used. It is based on the mathematical development by Aguilar, Balslev, and Combes [26,27] as well as Simon [28]. The application of this method leads in practice to a simple but powerful modification of the Hamiltonian $\hat{H}$ in Eq. (3),

$$\hat{H}(\theta) = \exp(-2\mathrm{i}\theta)\hat{T} + \exp(-\mathrm{i}\theta)\hat{V}. \tag{8}$$

In Eq. (8), $\hat{T}$ and $\hat{V}$ are the usual kinetic and potential energy operators of He, respectively. The complex-scaling angle θ can in principle be chosen arbitrarily within $0^\circ \leqslant \theta \leqslant 45^\circ$. In the limit of an infinite basis, all observables calculated with the aid of complex scaling should become independent of θ. Since only finite basis sets can be applied in practice, only approximate eigenstates can be obtained that may depend on θ. The angle θ can thus be understood as a variational parameter that modifies the adopted basis as can be seen from the inverse relation between basis-set exponents and the scaling angle discussed, e.g., in [29]. A diagonalization of the Hamiltonian (8) in the basis described by Eqs. (4) and (5) yields the complex-scaled energies $E_j(\theta)$ and wave functions $\Psi_j(\theta)$, where the latter are still defined by Eq. (6), but with complex coefficients $c_{jk}(\theta)$.

With the aid of the complex-scaled energies and wave functions, the transition-probability density into the electronic continuum can be extracted from the complex-scaled resolvent according to [9]

$$P(E, \theta) = \frac{1}{\pi}\mathrm{Im}\left\{\sum_k \frac{\langle \Psi_i^{T^-}(\theta^*)|\Psi_k^{He}(\theta)\rangle\langle\Psi_k^{He}(\theta^*)|\Psi_i^{T^-}(\theta)\rangle}{E_k^{He}(\theta) - E}\right\}. \tag{9}$$

The $\langle\Psi(\theta^*)|$ is the biorthonormal eigenstate to $|\Psi(\theta)\rangle$. It is obtained from the latter by a transposition and complex conjugation of the angular part, while the radial part is only transposed but not complex conjugated. The sum over

k includes all complex-scaled eigenstates and eigenvalues calculated by solving the generalized complex symmetric but non-Hermitian eigenvalue problem. As discussed above, in the limit of exact eigenstates, the density $P(E,\theta)$ becomes independent of the complex-scaling parameter θ. A variation of θ for approximate eigenstates provides the possibility of determining an optimal $\theta_{\rm opt}$ with highest stability. The best approximation of $P(E,\theta)$ is then obtained according to

$$\left.\frac{\partial P(E,\theta)}{\partial\theta}\right|_{\theta_{\rm opt}} = \text{min.} \rightarrow \; P(E) := P(E,\theta_{\rm opt}). \tag{10}$$

Furthermore, the θ dependence of the spectra gives an indication of the convergence of the results.

III. RESULTS

In Table I, the calculated transition probabilities for 15 ^1S bound states of He are listed. The results reveal that almost every second T^- decay will end in the first excited state of He. The next probable final state is the He ground state with nearly 23%. With a summed probability of 0.45%, the higher excited He states are rarely populated after β decay of T^-. Starting from the state $n=4$, the population decreases monotonically with n, the decrease becoming smaller with increasing n. The very small value found for the population of the second excited state ($n=3$) appears to be the result of an almost perfect cancellation of positive and negative contributions to the overlap integral due to the nodal structure of the final state. It is very sensitive to the proper description of the T^- ground state and is not reproduced within the Hartree-Fock approximation. In fact, Hartree-Fock predicts a continuously decreasing population starting from $n=1$ and thus a probability distribution more similar to the one of neutral tritium atoms.

TABLE I. Population probabilities P_n of the ^1S bound states of helium after the β decay of a T^- anion. Also given are the corresponding energies E_n (in atomic units) obtained in the present work.

n	E_n (This work)[a]	P_n (%) (This work)	P_n (%) (Ref. [18])	P_n (%) (Ref. [19])
1	**−2.903**4572	22.98998	22.993764	19.147
2	**−2.1459**527	46.86960	46.867404	21.149
3	**−2.0612**659	0.01320	0.013503[b]	0.27
4	**−2.03358**41	0.18363	0.210424	0.143
5	**−2.02117**49	0.09220	–	0.07
6	**−2.01456**04	0.05262	–	0.039
7	**−2.01062**35	0.03275	–	0.024
8	**−2.00809**09	0.02175	–	0.016
9	**−2.00636**79	0.01522	–	0.011
10	**−2.00514**07	0.01111	–	0.008
11	**−2.00423**55	0.00848	–	–
12	**−2.00355**07	0.00666	–	–
13	**−2.00302**05	0.00513	–	–
14	**−2.002**5951	0.00469	–	–
15	**−2.0022**570	0.00273	–	–
$\sum P_n$		70.30975	70.085095[b]	40.877

[a]The bold digits agree with the results in Ref. [30].
[b]Note, Ref. [18] reports $(0.0116204)^2 \approx 0.00135$ instead of $(0.0116204)^2 \approx 0.000135$. The latter value is used in this table.

The sum over all calculated bound states yields 70.3%. The summation over all calculated states (discrete and discretized continuum states) yields the expected value of 100.00%, since the same basis is used for initial and all final states, but indicates the proper numerical implementation. The excellent agreement of the energy eigenvalues at the order of μhartree with the very accurate data in [30] ensures, on the other hand, the high quality of the basis set adopted in the present work and its ability to describe many states simultaneously with high precision. A closer view of the energies shows that the degree of accuracy of the present results follows the expected trends. First, the accuracy increases with n, since the importance of the correlation decreases if the state becomes more asymmetric and the two electrons have smaller spatial overlap. For even higher values of n, the states become increasingly diffuse and thus it is very difficult to describe them properly without running into numerically caused linear dependencies.

A comparison with the final-state probabilities reported by [18] and [19] is also given in Table I. Especially for the highly populated ground and first excited states, the results of this work confirm the expectedly very accurate results of [18], which were obtained with explicitly correlated basis functions. For the second excited state, the agreement is still within a relative accuracy of 2.5% if an apparent typographical error in [18] is corrected. The agreement for the third excited state ($n=4$) is, however, less good (relative deviation of about 12%), but is of the same order of magnitude. In view of the very good agreement of the energy of the third excited state with the very accurate calculation in [30], the present result is expected to be reliable, but without the knowledge of the corresponding energy obtained by Frolov [18], it is impossible to finally decide whether the present transition probability or the one in [18] is more accurate.

The comparison with the results in [19], which were obtained with a relativistic multiconfiguration Dirac-Fock (MCDF) method shows, on the other hand, pronounced differences. The deviation is most remarkable for the first excited state, which according to the present work and [18] should be populated with about 47% probability and thus should clearly dominate the final-state distribution. However, in the MCDF results in [19], its probability is found to be about 21%. For the other states, except $n=3$, the results in [19] are always smaller than the present ones. The deviation increases rather uniformly from about 17 to 28% for n varying between 1 and 10. Since relativistic effects are expected to be small for light nuclei like T^- and ^{3}He, it appears very likely that the main reason for the difference of the results in [19] to the present ones (as well as the ones in [18]) is due to the small number of configurations used in the MCDF method compared with the present full CI method. Unfortunately, no details (such as energies) of the MCDF calculation in [19] are available to further clarify this issue, but any realistic estimate of the size of relativistic effects excludes their responsibility for the large discrepancy between the results in [19] compared to the non-relativistic calculations of this work or the one in [18].

The calculated transition-probability density into the electronic continuum of ^{3}He is presented for three different

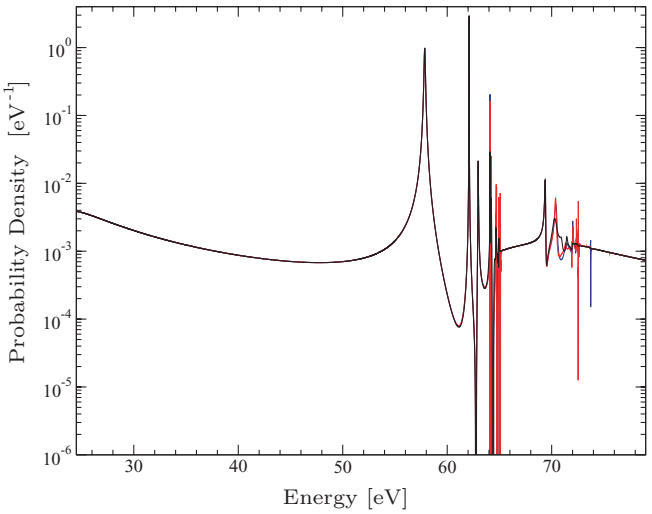

FIG. 1. (Color online) Final-state continuum probability density of He after β decay of T^- for $\theta = 24°$(red), $30°$(blue), and $36°$(black). (The energy scale is given relative to the He ground state.)

complex-scaling angles ($\theta = 24°$, $30°$, and $36°$) in Fig. 1. The overall spectrum is practically independent of θ. This indicates the high quality of the adopted basis set also for describing the electronic continuum. As is usually the case, (higher lying) resonances are most sensitive to the choice of θ. This is because it is difficult to find a single value of θ that is equally appropriate for describing a certain resonance and the underlying background continuum.

The continuum probability density is dominated by a peak corresponding to the first doubly excited singlet state $2s^2$. About 19% of the T^- decay ends up in the energy interval between 54.5 and 60 eV. Above the 65.4 eV threshold, the higher-lying doubly excited states $2sns$ and in the regime up to 79 eV (with diminishing importance) the $3sns$ peaks can be identified. The complex-scaling method provides the probability density $P(E)$ at any value of E and thus as a continuous function. In view of the sharp resonant structures and in accordance with the experimental needs, the final-state distribution is given in a discretized form as in [15]. For this purpose, the probability distribution $P(E)$ has been divided into small bins covering an energy range of 1.0 eV (up to a transition energy of 78.59 eV), 5.0 eV (from 78.59 to 214 eV), and 40.0 eV (from 214 to 904 eV). For each bin, the average excitation energy E_i and the integrated transition probability $P(E_i)$ were calculated and are given in Table II.

For the high-energy continuum states (above 904 eV), an approximate model tail is introduced, similar to the case of T_2 [12,15]. However, the situation is more complicated for T^-. In T_2 β decay, the high-energy tail was derived based on the idea that for sufficiently large energies of the escaping (formerly bound) electron, the effective potential of the remaining $^3HeT^{2+}$ ion can be well approximated by a point charge $Z = 2$. In fact, the remaining electron and tritium nucleus may be viewed as pure spectators, and thus

TABLE II. Discretized final-state probability distribution $P(E_i)$ for He following the β decay of a T^- anion. The mean excitation energies E_i are given relative to the ground state of ^{3}He.

E_i (eV)	$P(E_i)$(%)	E_i (eV)	$P(E_i)$(%)	E_i (eV)	$P(E_i)$(%)	E_i (eV)	$P(E_i)$(%)
25.084	0.36869	50.096	0.07054	75.086	0.09926	186.05	0.00960
26.081	0.32908	51.097	0.07403	76.085	0.09172	191.06	0.00873
27.081	0.28924	52.100	0.08005	77.085	0.08480	196.06	0.00796
28.081	0.25425	53.104	0.09041	78.086	0.07863	201.06	0.00727
29.082	0.22462	54.112	0.10943	80.950	0.31969	206.07	0.00666
30.082	0.19976	55.125	0.14982	85.967	0.23208	211.08	0.00612
31.083	0.17887	56.158	0.26863	90.980	0.17471	232.06	0.03471
32.084	0.16126	57.305	1.44117	95.991	0.13529	272.24	0.01998
33.084	0.14632	57.863	16.80345	101.00	0.10714	313.03	0.01250
34.085	0.13358	58.911	0.15914	106.01	0.08644	352.94	0.00832
35.085	0.12267	59.972	0.02281	111.01	0.07084	392.90	0.00581
36.085	0.11328	61.109	0.00924	116.02	0.05883	433.04	0.00421
37.086	0.10517	62.095	3.16161	121.02	0.04942	472.98	0.00314
38.086	0.09816	63.026	0.13662	126.03	0.04194	513.67	0.00239
39.087	0.09209	64.113	0.13095	131.03	0.03590	553.22	0.00186
40.087	0.08684	65.091	0.09512	136.03	0.03098	591.30	0.00148
41.088	0.08233	66.100	0.11217	141.03	0.02692	630.58	0.00119
42.088	0.07847	67.099	0.12245	146.04	0.02355	654.79	0.00101
43.089	0.07523	68.105	0.13639	151.04	0.02071	664.12	0.00089
44.089	0.07256	69.171	0.26130	156.04	0.01832	663.99	0.00081
45.089	0.07046	70.210	0.20446	161.04	0.01629	666.03	0.00073
46.085	0.06892	71.109	0.10126	166.05	0.01454	688.91	0.00063
47.084	0.06803	72.101	0.12307	171.05	0.01303	776.21	0.00048
48.090	0.06792	73.077	0.12211	176.05	0.01173	1550.1[a]	0.00358[a]
49.098	0.06870	74.083	0.10784	181.05	0.01059	$\sum P(E_i)$	29.65399

[a]For energies above 904 eV, the model tail in Eq. (13) was used.

the transition probability should approach for high energies the one obtained for a β-decaying tritium *atom* for which an analytical result is known. Due to the existence of two equivalent electrons, the atomic result is simply multiplied by a factor of 2 [12].

While for T_2, a hydrogenic wave function is a reasonable first-order approximation for the initial state, this is not the case for T^-. In fact, within independent-particle models, T^- is unstable. As a consequence, the fast electron in the final state may be well represented by a Coulomb wave function for a point charge $Z = 1$ (formed by the remaining He^+ ion), but the modeling of the initial state is less obvious within an independent particle model. This is also evident from the alternative point of view that a description of the remaining T nucleus and bound electron as a spectator would correspond for the active electron to an initial state with $Z = 0$ and thus no bound state. In order to obtain an atomic-like high-energy tail, the initial state is thus modeled as a hydrogen-like state with variable exponent. This exponent is then obtained by fitting the model spectrum to the *ab initio* spectrum of the full two-electron calculation in the energy range between 500 and 10 000 eV.

The initial T^- ground-state wave function (omitting the spin part for better readability) is then approximated as

$$\left|\tilde{\Psi}_i^{T^-}\right\rangle = |1s^{Z_e}1s^{Z_e}\rangle, \tag{11}$$

where $\langle \mathbf{r}|1s^{Z_e}\rangle$ is an STO with $(n, l, m) = (1, 0, 0)$, i. e., an atomic hydrogen $1s$ orbital with effective charge Z_e. In the spirit of the sudden approximation, the spectator electron remains in its orbital, and the final state of the He^+ ion is modeled as

$$|\tilde{\Psi}^{He}(E)\rangle = 2^{-\frac{1}{2}}[|1s^{Z_e}\phi_c(E)\rangle + |\phi_c(E)1s^{Z_e}\rangle], \tag{12}$$

where $|\phi_c(E)\rangle$ is the Coulombic continuum wave function for energy E and charge $Z = +1$. Using these model wave functions, the analytic expression

$$\tilde{P}(Z_e, E) = 2\left(\frac{8(1-Z_e)Z_e^{3/2}e^{-2\frac{\arctan(\kappa/Z_e)}{\kappa}}}{\sqrt{1-e^{-\frac{2\pi}{\kappa}}}\left(\kappa^2+Z_e^2\right)^2}\right)^2 \frac{dE}{\mathrm{Ry}}, \tag{13}$$

with $\kappa = \sqrt{(E+2)/\mathrm{Ry}}$ and $1\mathrm{Ry} = 13.60585972$ eV, is obtained for the probability density, i. e. for the model tail for the high-energy continuum states. A fit to the *ab initio* spectrum yielded $Z_e = 1.3074$. As is evident from (13), the probability density decays exponentially for high energies, which is the most essential property. (In fact, it has been verified that all subsequent conclusions are unchanged if a different model tail is used in which the initial-state charge is fixed to that of the tritium nucleus ($Z = 1$) and the effective charge of the final Coulomb wave is used as the fit parameter.)

Figure 2 compares the calculated final-state probability density with the analytical model tail and confirms the applicability of the latter for high energies, in fact already starting from about 200 to 250 eV, similarly as for T_2. The range of good agreement with a relative error of less than 5% extends to energies of 20 keV and thus far beyond the validity of the sudden approximation itself. Note, this energy is also much larger than the 10 keV used as an upper limit in the fit. The integrated probability density (including the model tail for energies above 904 eV) yields a total probability of 29.65% for ionization of He following β decay of T^-.

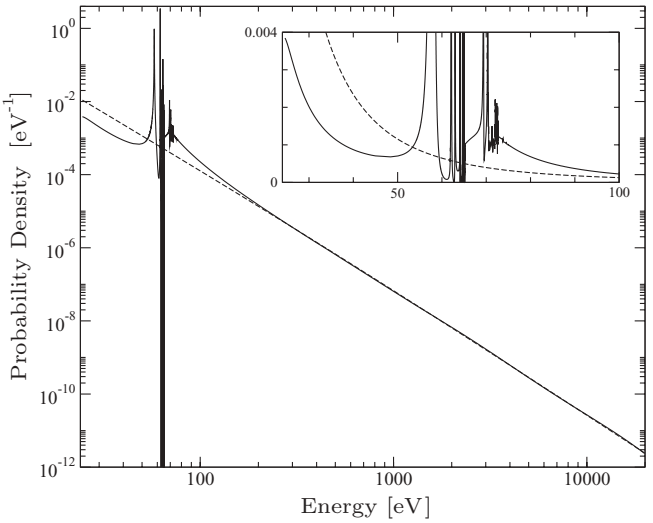

FIG. 2. Final-state continuum probability density of He after β decay of T^- (solid) and a model tail with $Z_e = 1.3074$ (dashed). The inset shows the probability density on a linear scale.

The mean excitation energy $\overline{E}$ relative to the electronic ground-state energy of T^- can be obtained from

$$\overline{E} = \sum_n E_n P_n + \int_{24.59\mathrm{eV}}^{904\mathrm{eV}} E\,P(E)\,dE + \int_{904\mathrm{eV}}^{\infty} E\,\tilde{P}(E)\,dE. \tag{14}$$

Insertion of the final-state probability distribution calculated in this work in (14) yields $\overline{E} = 27.487$ eV for the mean excitation energy of the decay product. This result may be compared to the one obtained by the alternative relation

$$\begin{aligned}\overline{E} &= \left\langle \Psi_i^{T^-}\middle|\hat{H}(\mathrm{He})\middle|\Psi_i^{T^-}\right\rangle \\ &= E_0(T^-) - 2\left\langle \Psi_i^{T^-}\middle|\frac{1}{r}\middle|\Psi_i^{T^-}\right\rangle.\end{aligned} \tag{15}$$

With the expectation value of $\langle r^{-1}\rangle$ and the ground-state energy $E_0(T^-)$ reported by Frolov in [18], the mean excitation energy calculated with (15) is $\overline{E} = 27.469$ eV. Frolov also reported the expectation values for the case of a finite mass of the tritium anion nuclei. Again using (15) for this case, one obtains $\overline{E'} = 27.479$ eV. This comparison confirms the quality of the final-state distribution obtained in this work and validates furthermore the use of the approximation of an infinitely heavy nucleus approximation.

Frolov noted in [18] that his calculated bound-state probability appears to imply a continuum contribution of about 30%. Since this value is about 10 times larger than the continuum probability known for neutral T atoms, he speculated that in fact a large number of decays (about 15–20%) may end up in triplet states of helium, leaving a much smaller fraction in the singlet continuum. The reasoning given in [18] is that the more diffuse ground state of T^- is not sufficient to explain such a large continuum contribution, as follows from a comparison with results obtained for Rydberg states of neutral T atoms. On the other hand, triplet states may be populated by the (virtual) interaction with the β electron omitted in the

sudden approximation. This argument is, however, erroneous. As has been discussed in detail in [22], the sum rule for the sudden approximation gives always unity, independently of higher-order corrections to it. This is also (as discussed above) fulfilled by the present calculation, which indeed confirms the about 30% continuum probability indirectly found but rejected in [18].

Finally, the exchange interaction is expected to be much smaller than the direct one (in [31] it was found for atomic tritium to be smaller by a factor of η^2), but already the direct term (first term beyond the sudden approximation) is by a factor of η^2 smaller than the sudden approximation. Close to the end point of tritium β decay one finds for the Sommerfeld parameter $\eta \approx -0.0271$ and for T_2 it was explicitly shown that the first-order correction to the sudden approximation is itself of the order of η^2 and thus of the order of 0.01% [12], in accordance with corresponding system-independent sum rules given in [22].

IV. CONCLUSION

In this work, the complete final-state probability distribution of He following the nuclear β^- decay of tritium anions has been calculated. For the small number of bound states considered previously in [18] the agreement is very good for the dominant ground and first excited states. The agreement with an earlier relativistic multiconfiguration Dirac-Fock calculation [19] is, on the other hand, very poor. Since such a large size of relativistic effects is not expected, especially not for the light nuclei involved, this deviation is attributed to a possibly too small basis set used in [19]. Nevertheless, the present study may stimulate further theoretical work to clarify the remaining discrepancies to [18] and of both works to the relativistic ones in [19].

In order to further test the accuracy of the present calculation, the bound-state energies were compared with very accurate literature data and were found to agree very accurately with them. Furthermore, the mean excitation energy obtained from the complete final-state spectrum was compared with the value predicted on the basis of closure. Again, very good agreement was found. Therefore, the results of this work should be reliable and of direct importance for the tritium neutrino-mass experiment KATRIN, which is presently under construction. To allow the use in the experimental analysis and for predicting how much a possible T^- admixture to the T_2 source spoils the extracted neutrino mass, the continuum transition probability is given in binned form, but it is also available numerically on request. Finally, it may be noted that a controlled admixture of T^- to the tritium source may in fact be used for the analysis of the experimental sensitivity to the atomic and molecular final-state spectrum.

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