Calculation of the β-Decay Spectrum of the T_2 Molecule beyond the Sudden Impulse Approximation

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The probability distribution of electronic excitations of HeT^+ following the β decay of the T_2 molecule has been calculated for the first time in the beyond sudden impulse approximation, removing the uncertainty related to the reliability of this approximation in connection with the neutrino mass experiments. Final state interactions are introduced to infinite order with respect to the decaying nucleus, and to first order with respect to all other particles, within the relativistic framework. The presented distribution features, in addition, corrections due to the nuclear motion, resonant structure and long tail (up to 800 eV) in the ionization continuum of HeT^+. [S0031-9007(96)01723-1]

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Six decades have elapsed since the time when W. Pauli suggested the existence of a hypothetical particle, the neutrino. Although the hypothesis has materialized, the particle itself has not—in the sense that its mass is still not determined. The experimental studies of β decay from molecular tritium have narrowed the upper bound for the mass of the electronic neutrino, which has been recently set to 4.3 eV [1]. However, the shadow of doubt has been cast on the interpretation of recent experiments, which *unisono* reveal an unphysical trend towards negative values of the square of the neutrino mass: $m_\nu^2 < 0$ [1–3]. The interpretation is very sensitive to the chemical effects disturbing the pure nuclear β-decay spectrum, and of major importance is the precise determination of the probability density for excitation of HeT^+ [4]. So far, this probability density has been available in the so-called sudden impulse approximation (SIA), which neglects the interaction of the β electron with the remaining molecule, except for the decaying nucleus. In this Letter, we present the first calculation which goes beyond SIA for the case of molecular tritium. Our treatment includes the bound states but emphasizes the excitations to the molecular continuum, as there are indications that this part of the spectrum is of particular importance regarding the "negative mass" issue [5].

The process under consideration is the β decay of one of the nuclei of molecular tritium (here assumed to be in the ground state) according to

$$T_2 \rightarrow HeT^+ + e + \overline{\nu}\,, \tag{1}$$

where the resulting daughter ion HeT^+ can be left in any of its rovibrational and electronic states, including the continua. Invoking charge-parity-time symmetries we concentrate on the transition matrix element for the collision problem with only two bodies in each channel: $T_2 + \nu \rightarrow HeT^+ + e$. Using the Born expansion, the transition matrix element is

$$\begin{aligned}\mathcal{T}_{fi} &= \langle \Phi_f | W_i | \Phi_i \rangle + \langle \Phi_f | U_f (E - H_f)^{-1} W_i | \Phi_i \rangle + \cdots \\ &\simeq \mathcal{T}_{fi}^{(0)} + \mathcal{T}_{fi}^{(1)}\,,\end{aligned} \tag{2}$$

where we have left out the second order term in weak interaction W_i (because of the smallness of the weak coupling constant g) and higher order Born terms. Φ_i is the channel eigenfunction describing the free motion of the initial molecule (T_2) and the neutrino, Φ_f is the channel eigenfunction in the final channel describing the molecular system HeT^+ and the ejected electron, and U_f describes the final channel (Coulombic) interaction given by

$$U_f = -\frac{Z_A e^2}{r_{\beta A}} - \frac{Z_B e^2}{r_{\beta B}} + \frac{e^2}{r_{\beta 1}} + \frac{e^2}{r_{\beta 2}}\,, \tag{3}$$

with $Z_B = Z_A = 1$. In the spirit of the two-potential formalism [6] we have excluded from U_f (part of) the Coulombic interaction between the β electron and the decaying nucleus labeled A. This particular choice of the interaction operator facilitates handling of the divergencies appearing in the *truncated* perturbation expansion of the transition amplitude (2) [7].

The transition probability considered here is $|\mathcal{T}_{fi}|^2 \simeq |\mathcal{T}_{fi}^{(0)} + \mathcal{T}_{fi}^{(1)}|^2 \simeq |\mathcal{T}_{fi}^{(0)}|^2 + 2\,\mathrm{Re}(\mathcal{T}_{fi}^{(0)} \mathcal{T}_{fi}^{(1)^*})$ as the term $|\mathcal{T}_{fi}^{(1)}|^2$ is partly canceled [8] by the interference terms involving the second order amplitude, $2\,\mathrm{Re}(\mathcal{T}_{fi}^{(2)} \mathcal{T}_{fi}^{(0)})$. A more complete treatment including $|\mathcal{T}_{fi}^{(1)}|^2$ is presented in Ref. [9]. The differential decay rate to the molecular state f can be obtained using the standard relation

$$w_{fi} = (2\pi/\hbar)\,|\mathcal{T}_{fi}(\mathbf{p}_\beta, \mathbf{p}_\nu)|^2 \delta(E_f - E_i)\,, \tag{4}$$

which means that the probability of the decay into the molecular channel with an electron energy within $E_\beta + dE_\beta$ (provided the neutrino has a momentum within $\mathbf{p}_\nu + d\mathbf{p}_\nu$ and all quantum numbers defining the molecular final state f are specified) is

$$dw_{fi} = w_{fi} dE_\beta d\mathbf{p}_\nu c^{-2} p_\beta E_\beta d\Omega_\beta\,, \tag{5}$$

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where $E_\beta^2 = \mathbf{p}_\beta^2 c^2 + m_e^2 c^4$ is the total relativistic energy of the β electron. The indices f and i stand for the triple quantum numbers $f \equiv \{n, J, \upsilon\}$ and $i \equiv \{0, 0, 0\}$ characterizing the electronic, rotational, and vibrational quantum numbers of the final and initial states, respectively. (Similarly, $j' \equiv \{n', J', \upsilon'\}$ will in the following characterize the intermediate states.)

To obtain the rate relevant for the experiment, the above expression has to be summed over the unobserved quantum numbers and other characteristics of the final state. In our case this entails the summation over quantum numbers n, J, and υ, integration over the momentum of the neutrino $\mathbf{p}_\nu$, integration over the *directions* Ω_β of the β electron, and summation over the spins (σ) of these particles. Generalizing the developments of Ref. [8] to the molecular case allows us to write the energy-differential decay rate as [9]

$$\frac{dw(E_\beta)}{dE_\beta} = \sum_n \frac{1}{2\pi^3 c^5} |T^{\rm nuc}|^2 |T^{\rm lep}|^2 p_\beta E_\beta [(\varepsilon - \overline{E}_{n0}^{\rm HeT^+})^2 - m_\nu^2 c^4]^{1/2} (\varepsilon - \overline{E}_{n0}^{\rm HeT^+}) \Theta(\varepsilon - \overline{E}_{n0}^{\rm HeT^+}) \times \Theta[(\varepsilon - \overline{E}_{n0}^{\rm HeT^+})^2 - m_\nu^2 c^4] \sum_{J,\upsilon} [|T_{fi}|^2 + 2\,{\rm Re}\{T_{fi}^{(0)} T_{fi}^{(1)^*}\}] \equiv \sum_n N_n(\varepsilon) I_n \,, \tag{6}$$

where

$$T_{fi}^{(0)}(\mathbf{K}) = \langle \psi_{nJ\upsilon}^{\rm HeT^+} | e^{i\mathbf{K}\cdot\mathbf{r}_{CA}} | \psi_{000}^{\rm T_2} \rangle \,, \tag{7}$$

$$T_{fi}^{(1)}(\mathbf{K}, E_\beta) = \sum_{j'=\{n'J'\upsilon'\}} \int \frac{d\Omega_\beta}{4\pi} \int_{\mathbf{q}} \frac{d\mathbf{q}}{(2\pi)^3} \frac{4\pi e^2}{q^2} F_{nn'}(\mathbf{p}_\beta, \mathbf{q}) M_{fi}(\mathbf{q}) T_{j'i}^{(0)}(\mathbf{K} + \mathbf{q}) \,, \tag{8}$$

with

$$F_{nn'}(\mathbf{p}_\beta, \mathbf{q}) = \frac{1}{\overline{E}_{nn'}^{\rm HeT^+} + E_\beta - E'_\beta + i\epsilon} \left(\frac{E_\beta + E'_\beta}{2E'_\beta} - \frac{\mathbf{p}_\beta \cdot \mathbf{q} c^2}{2E_\beta E'_\beta} \right) \tag{9}$$

and

$$M_{fi}(\mathbf{q}) = \langle \psi_{nJ\upsilon}^{\rm HeT^+} | \sum_{k=1}^{2} e^{-i\mathbf{q}\cdot\mathbf{r}_{Ck}} - \sum_{\mathcal{K}=A}^{B} Z_{\mathcal{K}} e^{-i\mathbf{q}\cdot\mathbf{r}_{C\mathcal{K}}} | \psi_{n'J'\upsilon'}^{\rm HeT^+} \rangle \,. \tag{10}$$

In the above equations, $\psi_{000}^{\rm T_2} = \varphi_0 \xi_{00}^0, \psi_{nJ\upsilon}^{\rm HeT^+} = \phi_n \chi_{\upsilon J}^n$ are the initial (T_2) and final (HeT^+) molecular states within the Born-Oppenheimer approximation, being products of the electronic wave functions φ_0, ϕ_n, and the corresponding rovibrational wave functions ξ_{00}^0, $\chi_{\upsilon J}^n$. $\mathbf{q} = \mathbf{p}_\beta - \mathbf{p}'_\beta$ is the momentum transfer between the intermediate and final states of the β electron. $\mathbf{K} = -(\mathbf{p}_\beta + \mathbf{p}_\nu)$ is the nuclear recoil, $\mathbf{r}_{CA}$ is the vector connecting the decaying nuclei with the molecular mass center, and $Z_{\mathcal{K}}$ is the charge of nucleus $\mathcal{K}$. Finally, $\mathbf{K} + \mathbf{q} = -(\mathbf{p}'_\beta + \mathbf{p}_\nu)$ is the (virtual) nuclear momentum recoil corresponding to the creation of the β electron in the intermediate state with momentum $\mathbf{p}'_\beta$ and energy E'_β.

In Eq. (6), $\overline{E}_{nn'} = \int_0^\infty [E_n(R) - E_{n'}(R)] |\xi_{00}^0(R)|^2 dR$ is an average energy difference between states n and n', while $\varepsilon = E_{\rm max} - E_\beta$, with $E_{\rm max} = T_{\rm max} + m_e c^2$ and $T_{\rm max}$ being the maximum kinetic energy of the β electron for $m_\nu = 0$. The factor $\frac{1}{(2\pi)^3}$ arises from the normalization of the plane waves, whereas the factor $\frac{4\pi e^2}{q^2}$ stems from the Bethe integration over the β-electron coordinate $\mathbf{r}_\beta$ in U_f-dependent matrix elements, resulting in the $e^{-i\mathbf{q}\cdot\mathbf{r}_{Ck}}$ and $Z_{\mathcal{K}} e^{-i\mathbf{q}\cdot\mathbf{r}_{CL}}$ terms of Eq. (10). The free wave channel functions were approximated by plane waves while performing the Bethe integration.

The leptonic matrix element $T^{\rm lep}$ with respect to the weak interaction W_i reduces to the so-called Fermi factor, equal to the product of the leptonic wave functions evaluated at the origin of the weak interaction, i.e., at $\mathbf{r}_{A\beta} = \mathbf{r}_{A\nu} = 0$.

To simplify presentation, we can outfactor from Eq. (6) the probability I_n for target excitation to the electronic state n, and structure it as

$$I_n = \sum_{J,\upsilon} [|T_{fi}^{(0)}|^2 + 2\,{\rm Re}(T_{fi}^{(0)^*} T_{fi}^{(1)})] = I^{(0)}(E_n) + I^{(1)}(E_n, E_\beta) \,. \tag{11}$$

Performing the summation over the rovibrational states belonging to the electronic final state n, and using the closure relation, the zeroth order contribution becomes

$$I^{(0)}(E_n) = \sum_{J,\upsilon} |T_{fi}^{(0)}(\mathbf{K})|^2 = \int_0^\infty |t_{n0}^{(0)}(R)|^2 |\xi_0|^2 \, dR \,, \tag{12}$$

which can be further approximated by the purely electronic overlap matrix element $t_{n0}^{(0)}(R_{\rm eff}) = \langle \phi_n(R_{\rm eff}) \,|\, \varphi_0(R_{\rm eff}) \rangle$ evaluated at the effective $R_{\rm eff} = \int_0^\infty R |\xi_0|^2 \, dR$ [10]. We have chosen to evaluate the electronic matrix elements at the effective distance $R_{\rm eff}$ optimized as to get the best match to the rovibrationally broadened bound state excitation probabilities of Ref. [11]. In this approximation, the total zeroth order transition probability still adds to 100%, while being independent of the recoil momentum.

We have shown [9] that after summation over $J, v; J', v'$ also the first order correction reduces to the **K**-independent electronic matrix element

$$I^{(1)}(E_n, E_\beta) = 2\,\mathrm{Re}\int \frac{d\Omega_\beta}{4\pi}\int_{\mathbf{q}} \frac{d\mathbf{q}}{(2\pi)^3}\,\frac{4\pi e^2}{q^2}\sum\!\!\!\!\!\!\int_{n'} F_{nn'}(\mathbf{p}_\beta, \mathbf{q})\,\langle\phi_n \mid \varphi_0\rangle^* \times\left\{\langle\phi_n|\sum_{k=1}^{2} e^{-i\mathbf{q}\cdot\mathbf{r}_{Ak}}|\phi_{n'}\rangle - \delta_{nn'}\langle\xi_{00}^0|\sum_{\mathcal{K}=A}^{B} Z_{\mathcal{K}}\,e^{-i\mathbf{q}\cdot\mathbf{r}_{A\mathcal{K}}}|\xi_{00}^0\rangle\right\}\langle\phi_{n'}\mid\varphi_0\rangle. \tag{13}$$

We are therefore able to concentrate on the effects of final state interactions, contained in electronic transitions. The effects of the recoil and the rovibrational broadening can then be studied separately by methods presented in Ref. [11].

While integrating over the virtual momentum transfer $\mathbf{q}$, only largest terms with respect to the Sommerfeld parameter $\eta = -\frac{e^2 m_e}{p_\beta}$ are retained (down to η^2), and we keep only the $L = 0$ component of the partial wave expansion of $e^{i\mathbf{q}\cdot\mathbf{r}}$. The latter restriction is correct as long as only the interference term $[2\,\mathrm{Re}(T_{fi}^{(0)^*} T_{fi}^{(1)})]$ is considered, because the following (4π) integration over the unresolved direction Ω_β of the β electron implies that all other contributions disappear independently of the exact nature (or symmetry) of the involved wave functions. Thus, for experiments not resolving the direction of the β electron, and when only the interference term is considered, the relevant excitations of HeT^+ are restricted to states of Σ symmetry [9].

After integration over $\mathbf{q}$ and Ω_β, and after taking the nonrelativistic limit, the first order correction (13) becomes [9]

$$I^{(1)}(E_n, E_\beta) = 2\,\mathrm{Re}\sum\!\!\!\!\!\!\int_{n'}\langle\phi_n\mid\varphi_0\rangle^*\langle\phi_{n'}\mid\varphi_0\rangle\left\{\langle\phi_n|\sum_{k=1}^{2}\left[-\eta^2\left(\frac{1}{2r_{Ak}} + \frac{r_{Ak}E_{nn'}^{\mathrm{HeT}^+}}{2}\right) - \eta i \ln r_{Ak}\right]|\phi_{n'}\rangle + \delta_{nn'}\langle\xi_{00}^0|Z_B\left[\eta^2\frac{1}{2r_{AB}}\right] + Z_A\left[\frac{4}{\pi}\eta + \frac{4}{3\pi}\frac{p_\beta}{E_\beta}\right]|\xi_{00}^0\rangle\right\}, \tag{14}$$

where we have omitted imaginary components of the nuclear contribution, since they do not contribute, if ξ_{00}^0 is a real function. Let us concentrate first on the nuclear contribution. It survives only when $n' = n$ and turns out to contain the contribution from the decaying nucleus (of order η) and the (previously unavailable for T_2) contribution from the spectator nucleus (of order η^2), both proportional to the sudden amplitude

$$I_{\mathrm{nuc}}^{(1)}(E_n, E_\beta) = \left(Z_A\frac{8}{\pi}\left[\eta + \frac{1}{3}\frac{p_\beta}{E_\beta}\right] + \eta^2 Z_B\langle\xi_{00}^0|\frac{1}{r_{AB}}|\xi_{00}^0\rangle\right)|\langle\phi_n\mid\varphi_0\rangle|^2. \tag{15}$$

The first term [where $Z_A = 1$ because of the splitting of U_f adopted in Eq. (3)] recovers the loss of zeroth order probability caused by evaluation of the Fermi factor for $Z_A = 1$ instead of $Z_A = 2$.

In the electronic contribution, the sum over intermediate states runs over the multiply degenerated continuum of ionized states of HeT^+, with different continuum branches starting at the excited states of HeT^{++}. To handle this situation, we use the complex coordinate based method (CCM) applied by us previously to the sudden impulse contribution (12) in Ref. [12]. To calculate the first order correction [Eq. (14)], we follow the development outlined in Ref. [13]. For excitations above the ionization threshold of HeT^+ the discrete index of I_n is changed to E. The electronic contribution can be structured as

$$\begin{aligned} I_{\mathrm{el}}^{(1)}(E, E_\beta) &= 2\,\mathrm{Re}\sum\!\!\!\!\!\!\int_{n'}\langle\varphi_0\mid\phi_n\rangle\langle\phi_n|D|\phi_{n'}\rangle\langle\phi_{n'}\mid\varphi_0\rangle \\ &= \{t_{n0}^{(0)^*} t_{n0}^{(1)} + \mathrm{c.c.}\} \\ &= \frac{1}{\pi}\,\mathrm{Im}\sum\!\!\!\!\!\!\int_n \frac{t_{n0}^{(0)^*} t_{n0}^{(1)} + \mathrm{c.c.}}{E - E_n + i\epsilon}, \end{aligned} \tag{16}$$

where $D(\overline{E}_{nn'}, E_\beta)$ stands for the operator whose definition is apparent from Eq. (14) and $t_{n0}^{(1)}$ is given by $t_{n0}^{(1)} = \sum_{n'}\langle\varphi_0\mid\phi_n\rangle\langle\phi_n|D|\phi_{n'}\rangle\langle\phi_{n'}\mid\varphi_0\rangle$. The imaginary component of Eq. (16) is evaluated by means of the CCM, applied here for the first time to interference terms of a scattering amplitude

$$I_{\mathrm{el}}^{(1)}(E, E_\beta) = \frac{1}{\pi}\,\mathrm{Im}\sum_{n,n'}\frac{\langle\varphi_0^{\theta^*}\mid\phi_n^\theta\rangle\langle\phi_n^{\theta^*}|D(\theta)|\phi_{n'}^\theta\rangle\langle\phi_{n'}^{\theta^*}\mid\varphi_0^\theta\rangle + \langle\varphi_0^{\theta^*}\mid\phi_{n'}^\theta\rangle\langle\phi_{n'}^{\theta^*}\mid D^*(\theta^*)|\phi_n^\theta\rangle\langle\phi_n^{\theta^*}\mid\varphi_0^\theta\rangle}{E - \mathcal{E}_n^\theta}, \tag{17}$$

where $\mathcal{E}_n^\theta$ are the complex eigenvalues of the dilated molecular Hamiltonian for HeT^+. The calculation has been performed in prolate spheroidal coordinates, in the clamped nuclei approximation at the nuclear separation R_{eff} discussed above, generalizing the numerical apparatus presented in Ref. [12] and doubling the basis sets. The calculation of the matrix elements with respect to the operator D [containing r, $\frac{1}{r}$, and $\ln(r)$ terms] has been reduced to two-dimensional integrations which are performed numerically.

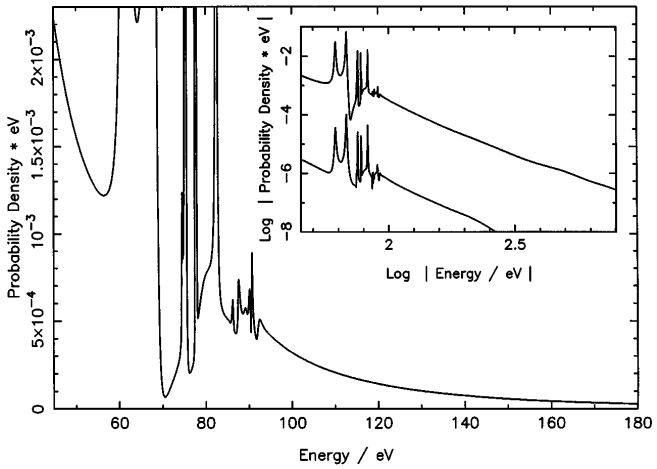

FIG. 1. The final distribution of the probability density in eV^{-1} [renormalized to $I^0(E)$] as a function of the excitation energy E of HeT^+, starting from the ionization threshold (i.e., at about 45 eV below the end point). In the insert, the first order correction $I^{(1)}_{el}(E)$ (lower curve) is compared to the zeroth order probability density $I^{(0)}(E)$ (upper curve), the logarithmic scale of energy covers 45 to 800 eV.

Analyzing the results, we first confirm the accuracy of the zeroth order treatment presented in Ref. [12] and extended here to an excitation range of 800 eV (see the insert in Fig. 1). Regarding the first order correction we note that both components of $I^{(1)}_{nuc}$ are only weakly dependent on the energy of the β electron (via η and η^2, respectively) and, as apparent from Eq. (15), depend on the excitation of HeT^+ only via the sudden amplitude. They will therefore not contribute significantly to the redistribution of probability in the renormalized spectrum. Such redistribution could still be induced by the electronic contribution $I^{(1)}_{el}$. This contribution is *a priori* of order η, considering complexity of the *molecular* scattering wave functions for HeT^+. However, our numerical results show surprisingly that also the electronic contribution turns out to be proportional to the sudden amplitude. This is visualized in the insert of Fig. 1 where $I^{(1)}_{el}$ is seen to be parallel to $I^{(0)}$ on a logarithmic scale.

This result, obtained here for the first time for the molecular decay of T_2, is therefore similar to the atomic case [14]. After renormalization of the corrected spectra, the redistribution of the excitation probability becomes negligible and does not influence the sudden impulse probability contained in the asymptotic tail, which according to our calculation is 0.25% in the range 165 to 800 eV. The precise determination of the asymptotic probability is important in view of recent suggestions that it considerably affects the neutrino mass extracted through the comparison of the experimental data with the theoretical distribution [5].

TABLE I. The three moments $S(n)$ $(n = 0, 1, 2)$ in $[eV]^{-n}$ of the first order corrected probability distribution compared to the corresponding values obtained within the sudden approximation (given in brackets).

	Bound states	44.8 to 164.2 eV	164.2 to 800 eV
$S(0)$	0.8565 (0.8565)	0.1382 (0.1382)	0.0027 (0.0027)
$S(1)$	8.5083 (8.5098)	9.5388 (9.5405)	0.7070 (0.7068)
$S(2)$	262.83 (262.88)	696.72 (696.89)	225.11 (224.91)

The final spectrum is presented in Fig. 1, and is also available in tabular form. To give the feel for the negligible size of the first order correction, in Table I we compare the first three moments of the sudden amplitude with their first order corrected (and renormalized) counterparts.

The particular advantage of the present approach is above the ionization threshold of HeT^+ and thus our new distribution is especially recommendable, if the mass extracting fitting procedure extends far away from the end point of the β spectrum. To assess the accuracy of our method, we have performed a calculation for the atomic case [9] reproducing the analytically available (sudden impulse) result with a relative accuracy better than 0.002% in the range up to 800 eV.

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