

## Probability Distribution of Excitations to the Electronic Continuum of $\text{HeT}^+$ Following the $\beta$ Decay of the $\text{T}_2$ Molecule

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We present a calculation of the probability density for the excitation to the molecular continuum of  $\text{HeT}^+$  following the  $\beta$  decay of  $\text{T}_2$ , pertinent to the investigation of chemical effects in the neutrino mass experiments. The relevant transition amplitude has been obtained by means of a novel technique that avoids the explicit calculation of the continuum states of  $\text{HeT}^+$ , and delivers the properly normalized probability density which includes both the background and resonant scattering contributions. We found two distinct sharp resonances at 75 eV below the end point of  $\beta$  spectrum where excess count rate has been observed in the recent neutrino mass experiment.

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The present study of the continuous spectrum of  $\text{HeT}^+$  is related to our previous work [1-7] on the chemical effects in the neutrino mass experiments [8-10]. In such experiments the spectrum of  $\beta$  electrons from tritium nuclei bound in  $\text{T}_2$  molecules is investigated. Since the decay energy of the free tritium nucleus is shared only between the  $\beta$  electron, the daughter nucleus  $^3\text{He}$ , and the neutrino, the  $\beta$  spectrum carries the information about the rest mass of the neutrino. However, the pure (i.e., bare-nuclei)  $\beta$  spectrum is deformed under experimental conditions by the environmental effects, since the decaying nucleus is a part of the  $\text{T}_2$  molecule which in turn enters a (frozen tritium) solid. Interaction with the hosting molecule and with the surrounding solid changes the energy of the expelled  $\beta$  electron. For example, the  $\text{T}_2$  molecule after decay is rearranged into the  $\text{HeT}^+$  molecular ion. Hence the amount of energy carried by the  $\beta$  electron depends on the final state of the  $\text{HeT}^+$  ion which can end up in any of its discrete states, or in the (electronic) continuum. A smaller fraction of the available decay energy is deposited in the solid via excitations of the surrounding  $\text{T}_2$  molecules. Therefore, in order to determine the mass of the neutrino, these molecular and solid state effects have to be taken into account. The smaller the neutrino mass, the higher the accuracy required for the theoretical description of these environment effects [4].

The problem of the molecular effects has been treated previously [1-5,11] and the solid state effects (in frozen tritium) were considered in Ref. [6]. However, the excitations to the electronic continuum have been addressed previously [7,11] only in a simplified manner. In Ref. [7] the energies and widths of the two strongest resonances in the continuum of  $\text{HeT}^+$  have been obtained and a model of the shakeoff probability density based on the simple Breit-Wigner formulation has been constructed. It has been shown that about two-thirds of all continuum exci-

tations concentrate in those two resonances near the ionization threshold of  $\text{HeT}^+$ . The resulting distribution proved to be much different from the one obtained previously by Martin and Cohen [11] by Stieltjes imaging technique. Although the Breit-Wigner distribution is believed to be reliable in the vicinity of the resonances, it treats the contribution from the scattering background and the interference effects in a rather oversimplified way. In the present contribution, we present a first principle, *ab initio* calculation of the probability density for the shakeoff to the molecular continuum of  $\text{HeT}^+$ , extracting it from the imaginary part of the resolvent.

The probability for the excitation to the electronic continuum of  $\text{HeT}^+$  following the  $\beta$  decay of  $\text{T}_2$  can be given (within the sudden impulse approximation) in terms of the overlap integral between the initial (ground) state of  $\text{T}_2$  and the final (continuum) state of  $\text{HeT}^+$ :

$$P(E) = |\langle \Phi_f^{\text{HeT}^+}(E) | \Phi_0^{\text{T}_2}(E_0) \rangle|^2. \quad (1)$$

Direct evaluation of this expression requires knowledge of the accurate solutions  $\Phi_f^{\text{HeT}^+}(E)$  from the continuum of  $\text{HeT}^+$ . These final wave functions ought to describe the doubly excited molecular continuum, together with all correlational intricacies leading to the presence of resonances. For this reason we have chosen a method which *avoids the explicit calculation of these functions*. The probability distribution is extracted as the imaginary part of the expectation value of the  $\text{HeT}^+$  resolvent operator with respect to the *ground state* of  $\text{T}_2$ . This method has been applied previously to the calculation of cross sections for atomic photoionization [12], two-photon ionization [13], and inelastic electron scattering on atoms [14]. The method is based on the observation that

$$P(E) = \pi^{-1} \text{Im}\{G(E)\}, \quad (2)$$

where  $G(E)$  is the (ground state) expectation value

defined by

$$G(E) = \lim_{\epsilon \rightarrow 0} \langle \Phi_0^{T_2} | (\hat{H}_{\text{HeT}^+} - E - i\epsilon)^{-1} | \Phi_0^{T_2} \rangle. \quad (3)$$

In the above expression  $\hat{H}$  is the total Hamiltonian of  $\text{HeT}^+$  and  $\Phi_0$  is the ground state of  $T_2$  (both in the clamped-nuclei approximation). Introducing the complete eigenstate expansion of the operator  $\hat{H}$ ,  $G(E)$  can be written as

$$G(E) = \lim_{\epsilon \rightarrow 0} \sum \int \frac{\langle \Phi_0^{T_2} | \Phi_n^{\text{HeT}^+} \rangle \langle \Phi_n^{\text{HeT}^+} | \Phi_0^{T_2} \rangle}{E_n - E - i\epsilon}, \quad (4)$$

where the symbol  $\sum \int$  abbreviates collectively the summation over the discrete part and integration over the continuous part of the spectrum of  $\text{HeT}^+$ . Using the well-known relation [15]

$$\lim_{\epsilon \rightarrow 0} \int_a^b \frac{F(E')}{E' - E - i\epsilon} dE' = \mathcal{P} \int_a^b \frac{F(E')}{E' - E} dE' + i\pi F(E), \quad (5)$$

one obtains for  $E > 0$ ,

$$G(E) = \sum_n \frac{\langle \Phi_0^{T_2} | \Phi_n^{\text{HeT}^+} \rangle \langle \Phi_n^{\text{HeT}^+} | \Phi_0^{T_2} \rangle}{E_n - E} + \mathcal{P} \mathcal{P}(G) + i\pi |\langle \Phi_f^{\text{HeT}^+}(E) | \Phi_0^{T_2}(E_0) \rangle|^2, \quad (6)$$

where  $\mathcal{P} \mathcal{P}(G)$  denotes the Cauchy principal part of the integral. Since the first two terms in the above expression are real, the imaginary part of  $G(E)$  gives the probability density  $P(E)$  as shown in Eq. (2). Therefore, this density can be obtained as the imaginary part of the ground state expectation value given by Eq. (3), provided that one can find a meaningful numerical approximation to the resolvent operator. If the continuum is discretized by introduction of a finite set of basis functions, the eigenvalue problem for  $\text{HeT}^+$  is brought to the matrix form

$$\mathbf{Hc}_n = E_n \mathbf{Sc}_n, \quad (7)$$

where the  $\mathbf{c}_n$  are the column vectors consisting of expansion coefficients in the basis  $\mathbf{h}$ ,

$$\Phi_n = \mathbf{hc}_n, \quad (8)$$

$\mathbf{S}$  is the overlap matrix, and  $\mathbf{H}$  is the matrix of the Hamiltonian  $H_{\text{HeT}^+}$ . The integration over the continuum given in expression (4) is changed into a discrete sum. But this straightforward procedure violates the analytical structure of the probability density which vanishes according to

$$P(E) = \frac{1}{\pi} \text{Im} \left\{ \sum_n \frac{\langle \Phi_0 | \Phi_n \rangle \langle \Phi_n | \Phi_0 \rangle}{E_n - E} \right\} = 0, \quad E_n \text{ real}. \quad (9)$$

However, if the probability density is first continued analytically by means of the complex coordinate method [12], its discretized approximation does not vanish,

$$P^\theta(E) = \frac{1}{\pi} \text{Im} \left\{ \sum_n \frac{\langle \Phi_0^{\theta*} | \Phi_n^\theta \rangle \langle \Phi_n^\theta | \Phi_0^\theta \rangle}{E_n^\theta - E} \right\} \neq 0, \quad (10)$$

$E_n^\theta$  complex.

Here the functions  $\Phi_n^\theta$  are the solutions to the *dilated* matrix eigenvalue problem,

$$\mathbf{H}(\theta) \mathbf{c}_i^\theta = E_n^\theta \mathbf{S} \mathbf{c}_i^\theta, \quad \Phi_n^\theta = \mathbf{hc}_i^\theta, \quad (11)$$

that is obtained from the original one via dilation of the Hamiltonian  $\hat{H} \equiv \hat{H}_{\text{HeT}^+}$ ,

$$\hat{H}(\theta) = \hat{U}(\theta) \hat{H} \hat{U}^{-1}(\theta), \quad \hat{U}(\theta) f(\mathbf{r}) = e^{3\theta/2} f(e^\theta \mathbf{r}), \quad (12)$$

where  $\theta = \alpha + i\beta$  is the dilation parameter. The bi-orthonormal functions  $\Phi_n^{\theta*}$  are obtained from the eigenvalue problem adjoint to the one in Eq. (11). It has been shown [12-14] that this procedure correctly recovers various characteristics of the continuous spectrum.

In the present context, the complex coordinate method can be seen merely as a technique that facilitates the performance of the limit procedure implied by Eq. (4). It converts a mathematically singular expression into one that is amenable to numerical computations. The probability density itself is *not* influenced by the dilation transformation. Indeed, noting that  $\hat{U}(\theta^*) = \hat{U}^\dagger(\theta)^{-1}$  [16] and using the fact that for a bound state  $\Phi_0(\theta) = U(\theta) \Phi_0$ , it is easily seen that

$$P^\theta(E) \equiv \pi^{-1} \text{Im} G^\theta(E) = \pi^{-1} \text{Im} \langle \Phi_0(\theta^*) | [\hat{H}(\theta) - E]^{-1} | \Phi_0(\theta) \rangle \quad (13)$$

$$= \pi^{-1} \text{Im} \langle U(\theta^*) \Phi_0 | U(\theta) (\hat{H} - E)^{-1} U^{-1}(\theta) | U(\theta) \Phi_0 \rangle \quad (14)$$

$$= \pi^{-1} \text{Im} \langle \Phi_0 | (\hat{H} - E)^{-1} | \Phi_0 \rangle = \pi^{-1} \text{Im} G(E) = P(E). \quad (15)$$

The above relation is valid for any dilation angle  $\theta$ . In practical applications  $\theta$  is chosen as to (a) expose the resonances of interest, and (b) assure the maximal stability of the probability density, as discussed below. The computation of the probability distribution  $P(E)$  has been reduced to the solution of the dilated matrix eigenvalue problems for  $T_2$  and  $\text{HeT}^+$ . Both calculations have been performed in the prolate spheroidal coordinates, using the clamped nuclei approximation (at the  $T_2$  equilibrium sep-

aration  $T=1.4$  bohr) and an explicitly correlated basis set. The details of this calculation were presented in Ref. [7], where we have also derived the appropriate (for the elliptical coordinate system) form of the dilation transformation, that is,

$$(\xi, \eta, \phi) \rightarrow (e^\theta, \xi, \eta, \phi). \quad (16)$$

We have also shown that this transformation is consistent

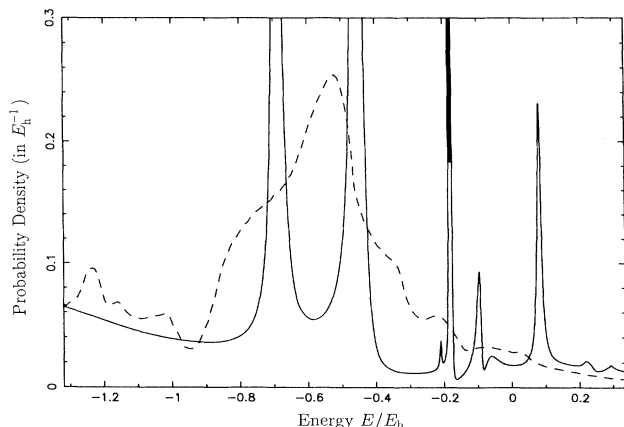


FIG. 1. Distribution of the probability density (in  $E_h^{-1} \equiv 1$  a.u. $^{-1}$ ) for the shakeoff to the electronic continuum of  $\text{HeT}^+$  following the  $\beta$  decay of  $\text{T}_2$ . —, present work; ---, results of Martin and Cohen [11], obtained by the Stieltjes imaging technique. The zero of energy corresponds to the breakup threshold of  $\text{HeT}^+$ , and our spectrum starts at  $E = -1.3185$  a.u. which is the ionization threshold for  $\text{HeT}^+$ . The  $\beta$  electron attains its maximal (end-point) energy when the  $\text{HeT}^+$  ends up in its ground state (here  $E_{\text{HeT}^+}^{\text{ground}} = -2.9780$  a.u.). The excitation energy with respect to that ground state is therefore reflected as the energy deficit of the  $\beta$  electron relative to the experimental end point.

with the use of the clamped-nuclei approximation, in the sense that the so-called outer scaling is not necessary. Still, however, the direct calculation of the matrix elements of the complex-dilated Hamiltonian in the explicitly correlated basis set is a very difficult task. For this reason these matrix elements have been calculated via an analytic continuation of their values for real dilation, using the least-squares polynomial technique. A more detailed discussion of this procedure will be given in a separate publication, and therefore we give here only a brief sketch of it.

First, a number of standard calculations of the Hamiltonian matrix are performed for different values of the (real) dilation factor  $\alpha$ . This can be done exactly via an inverse scaling of the corresponding nonlinear parameters in the basis functions. The matrix elements corresponding to different  $\alpha_i$  values,  $i=1, \dots, N_\alpha$ , are stored. This amounts to  $N_\alpha$  arrays of length  $M = N(N+1)/2$ , with  $N$

TABLE I. Basis-set description.

	$\xi_1$	$\xi_2$	$\eta_1$	$\eta_2$
$\text{T}_2$	0.781 32	0.305 32	0.336 00	0.132 00
$\text{HeT}^+$ (basis 1)	1.297 60	0.682 40	0.461 00	0.000 00
$\text{HeT}^+$ (basis 2)	1.452 00	0.535 64	0.226 00	0.310 80

being the dimension of the basis set. In this calculation  $N_\alpha=7$  has been chosen, where  $\alpha$  varies between 0.97 and 1.03. Using a simple polynomial least-squares fit, every configuration interaction matrix element  $h_{i \geq j}$  is expressed as a polynomial in  $\alpha$ :

$$h_{i,j} = p_{i,j}^n(\alpha) = \sum_{k=0}^n c_k \alpha^k, \quad (17)$$

where  $n$  denotes the order of the polynomial (here  $n=4$ ). The matrix representation of the complex-dilated Hamiltonian is now available by calculation of the polynomials  $p_{i,j}(\alpha)$  at complex arguments.

Once the complex matrix elements are obtained, the eigenvalue problems for  $\text{T}_2$  and  $\text{HeT}^+$  are solved, and the probability density  $P(E)$  is calculated according to Eq. (10). The summation includes all complex eigenvalues of the dilated  $\text{HeT}^+$  eigenvalue problem. Most of them correspond to the transformed continuous spectrum of  $\text{HeT}^+$ , while some of them correspond to resonances. The character of the eigenvalues (resonant or continuum) can be recognized from their behavior as a function of the dilation parameter  $\theta$ , but this distinction is not essential from the point of view of the probability density calculation. The interaction between the resonant and non-resonant (background) contributions is automatically included. An important feature of our method is that it delivers absolute values of  $P(E)$ , i.e., the probability density is automatically normalized.

The resulting probability density  $P(E)$  is presented in Fig. 1. In this calculation 100 basis functions for the  $\text{T}_2$  molecule and 200 basis functions for the  $\text{HeT}^+$  have been used. The nonlinear parameters in the basis sets are listed in Table I. These values have been established by optimizing the real stabilization graph. The investigation of the stability of the resonant roots with respect to the complex scaling parameter  $\theta$  allowed the calculation of positions and widths of the resonances of  $\text{HeT}^+$ , given in Table II.

TABLE II. Resonance of  $\text{HeT}^+$ .

Resonance No.	Position (in a.u.)	Width $\Gamma$ (in a.u.)	Height (in a.u. $^{-1}$ )	Transition probability	Basis set No.
1	-0.688 14	0.024 29	0.7600	0.029	1
2	-0.451 15	0.018 76	1.6289	0.048	1
3	-0.209 93	0.005 09	0.0250	0.0002	2
4	-0.185 14	0.003 75	0.3395	0.002	2
5	-0.177 11	0.002 94	0.6496	0.003	2

Using 100 energetically lowest lying states of  $\text{HeT}^+$  the probability density spectrum has been calculated for different values of the complex scaling parameter  $\theta$ . Because of the finite basis set, the spectrum is not totally  $\theta$  independent. To receive the final spectrum we have used the criterion of its optimal stability [ $dP(E)/d\theta = \min$ ] implemented as follows: In the region between the ionization threshold and the lowest lying resonance the range of angles giving a most stable spectrum has been chosen. In the following resonant region (containing the four lowest lying resonances) the scaling factor  $\theta$  has been chosen so as to achieve the best stability of the resonant eigenvalues. The region starting from  $-0.19$  a.u. is represented by the scaling factor that represents the fifth resonance and the background in a most stable way. The area under the curve is equal to 0.1277 in the displayed energy range (without any additional normalization), compared to 0.1348 obtained by Martin and Cohen [11]. Their spectral distribution has been obtained by Stieltjes imaging, and shows much less pronounced structure than ours. Our method allows *ab initio*, first principles calculation of absolute transition probabilities in the continuum, including both the background scattering contribution and the fine structure of the spectrum (including the line shapes) caused by existence of resonances.

From the displayed spectrum and the values of the transition probability one can clearly see the importance of the five lowest lying resonances (see Table II) that absorb most of the continuum excitations. In addition to the dominant contributions from the  $^1\Sigma^+$  ( $\sigma^2$ ) and ( $2\sigma3\sigma$ ) resonances, also contributions from higher lying, closely spaced (and therefore strongly interacting) resonances are observable. Interestingly, we notice very sharp resonances of bound-state character at 75 eV above the ground state of the  $\text{HeT}^+$  molecular ion, i.e., in the exact vicinity of the "missing spectral component" observed by Weinheimer *et al.* [10] at 75 eV below the end point of the experimental  $\beta$  spectrum.

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