

**Molecular Effects in the Neutrino Mass Determination
From Beta-Decay of The Tritium Molecule**

O.Fackler^{a,b}, B.Jeziorski^c, W.Kolos^c, H.J.Monkhorst^d,
M.Mugge^a and K.Szalewicz^c

a Lawrence Livermore National Laboratory, University of California,
Livermore, California 94550, USA

b Department of Physics, The Rockefeller University,
New York, New York 10021, USA

c Quantum Chemistry Laboratory, Department of Chemistry,
University of Warsaw, 02-093 Warsaw, Poland

d Quantum Theory Project, Departments of Chemistry and Physics,
University of Florida, Gainesville, Florida 32611, USA

Abstract

Molecular final state energies and transition probabilities have been computed for beta-decay of the tritium molecule. The results are of sufficient accuracy to make a determination of the electron neutrino rest mass with an error not exceeding a few tenths of an electron volt. Effects of approximate models of tritium beta-decay on the neutrino mass determination are discussed

I. Introduction

Experiments are being prepared or performed in several laboratories aiming at electron neutrino mass determination from measurements of the tritium β -decay spectrum near the endpoint. These experiments can be separated into (1) those dealing with atomic, molecular or solid state tritium, and (2) those in which the decaying tritons have a more complex molecular or solid state surrounding. Only in the first case can one perform reliable quantum mechanical computations for the final states of the daughter system, and therefore only in these experiments will the accuracy of the neutrino mass determination depend solely on the experimental resolution. In the second group of experiments the inherently less accurate theoretical results for the final states will always introduce an additional uncertainty into the determined value of the neutrino mass.

In the present paper we give a summary of our accurate theoretical treatment of molecular effects ¹⁻⁶ accompanying the β -decay of T_2 . We consider transitions to the electronic ground state of HeT^+ , to excited bound states of this ion, as well as to the resonance and scattering states. In the case of transitions to lowest electronic states we explicitly consider excitations to all possible rovibrational (rotational and vibrational) states. These results are used to construct the Kurie plots and to perform numerical experiments that show the magnitude of error in the neutrino mass determination arising if the accurate treatment of the final states is replaced by a more approximate one. We also discuss the solid state effects in frozen T_2 and show that they are either small or computable.

The results presented below will be used to interpret the data from the frozen tritium experiment now under way at LLNL (see the accompanying contribution in these proceedings).

II. Kurie plots and their accuracy

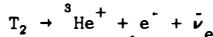
It is well known that to extract the neutrino rest mass from the β -decay spectrum one must compute the Kurie plots ⁶ defined as

$$K(E; m_\nu) = \left[\sum_n P_n K_n^2(E; E_n, m_\nu) \right]^{1/2} \quad (1)$$

$$K_n(E; E_n, m_\nu) = (m_\nu + E - E_n)^{1/2} [(m_\nu + E - E_n)^2 - m_\nu^2]^{1/4} \quad (2)$$

where E denotes the β -electron energy relative to the endpoint energy, m_ν the neutrino rest mass, P_n the transition probability to the n -th final state of the daughter ion, and E_n the energy of this final state measured relative to the lowest state energy.

The process under consideration is



Since the ground state of T_2 is a ${}^1\Sigma_g^+$ state, n in Eq.(1) labels all ${}^1\Sigma$ rovibronic (rotational, vibrational and electronic) states of the ${}^3\text{He}^+$. The values of E_n and P_n for all these states are needed to calculate the Kurie plots (1).

The following basic methods and techniques have been applied in our work to provide the necessary input for the Kurie plots:

1. First-order time-dependent perturbation theory,
2. Neglect the β -electron interaction with the molecular electrons,
3. Adiabatic approximation,
4. Expansion of the electronic wavefunction in elliptic coordinates,
5. Numerical solution of the vibrational equation.

Since we do not use any new approaches we will not present the details of the above steps 1-5, and only their accuracy and reliability will be discussed:

1. The applicability of first-order perturbation theory follows from the smallness of the weak interaction operators.

2. In this Born approximation one essentially neglects the following effects: (a) screening of the active nucleus and the final state dependence of this screening, (b) exchange of the β -electron with the molecular ones, (c) correlation of the β -electron in its continuum orbital with the bound state electrons. Since in the case of tritium decay the momentum of the β -electron is relatively large, all three effects should be small, with effect (a) being probably the largest one. It has been shown that for the two lowest states of the T atom the effects (a) and (c) change the transition probability by only 0.17%. There is no reason to suppose that the molecular binding in T_2 may change this value significantly.

3. The adiabatic approximation consists of factoring the molecular wavefunction into electronic and rovibrational wavefunctions. For the ground states of T_2 and ${}^3\text{He}T^+$ one may expect⁸ the relative value of the nonadiabatic effects in the energy to be less than 10^{-6} . They may be larger for some higher excited states but since the transition

probabilities to these states are considerably smaller than to the ground state we conclude that the adiabatic approximation is very reliable.

4. The expansion of the electronic wavefunction in terms of the basis set expressed in elliptic coordinates and depending explicitly on the interelectronic distance (r_{12}^n , with $n < 4$) is known to be very rapidly converging (see Ref.1 and references therein). Most of our computations have been carried out with 200-term expansions and the results indicate that for a few lowest bound states the error in the probabilities is approximately 0.00001. The error may be larger for high lying Rydberg states and also for the resonance states. We have shown, however, by performing numerical experiments, that this effect has no effect on our final results relevant to the neutrino mass determination.

5. The vibrational equation has been solved numerically for all bound rovibrational and continuum states² resulting from the nuclear motion in the electronic states 1-4 and 6. Using sum rules we have shown that for each considered electronic state of ${}^3\text{HeT}^+$, and a given rotational quantum number j , the error in the transition probabilities summed over the whole spectrum amounts to less than 0.0001.

Concluding this section we can say that in our computation of the Kurie plots for the T_2 molecule the largest error arises from approximations 1 and 2, but not from molecular computations. In our opinion, the accuracy of the Kurie plots for molecular T_2 computed in the present work is equally as accurate as that which can be calculated for atomic T.

III. Computation of wavefunctions and of transition probabilities

For the electronic ground state of T_2 we have used the previously determined wavefunctions^{9,10} different for different regions of the internuclear distance. For ${}^3\text{HeT}^+$ six lowest electronic states have been considered explicitly. For each of these states a selection of terms in the expansion of the electronic wavefunction has been made and the nonlinear parameters have been optimized. Transition probability to the electronic ground state of ${}^3\text{HeT}^+$, computed for the equilibrium internuclear distance in T_2 , $R = 1.4$ bohr, amounts to 58.2%, and to the five lowest excited states 26.4%. By diagonalizing the Hamiltonian matrix we get, however, more eigenvalues below the ionization continuum. With our best 249-term wavefunction we obtained 16 states in this region. Transition probabilities to the 10 highest of these states, for which the nonlinear parameters in the wavefunctions have not been individually optimized, sums

to 1.1%. Thus the total transition probability to all bound excited states is 27.5%.

For resonance states the energies have been computed using the stabilization method.¹¹ The reliability of this method has been demonstrated by performing (in elliptic coordinates) computations for the united atom as well as for the separated atoms, and reproducing the corresponding atomic resonance energies.^{4,5}

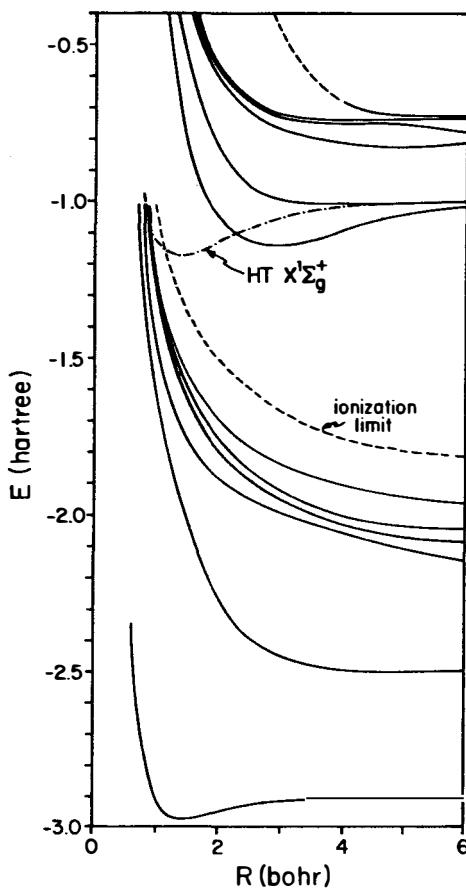


Fig. 1. Potential energy curves for HeT^+

The transition probability to all resonance and scattering states in the continuum, amounts to 14.3%. In our most accurate computations we have used 249 terms in the expansion of the H matrix, and the sum of transition probabilities to all these 249 states amounts to 1.00000.

Some of the computed potential energy curves are shown in Fig. 1. The equilibrium internuclear distance for T_2 is 1.4 bohr, and due to the slow motion of the nuclei the transitions to the various electronic states of HeT^+ occur without any change of R (Franck-Condon-type transitions). It is seen in Fig. 1 that only transitions to the ground state can end up in a stable rovibrational state of the daughter molecular ion. For all other states the internuclear distance $R = 1.4$ bohr corresponds to a

strongly repulsive part of the potential energy curve and no stable vibrational states are possible.

To compute the transition probabilities to the rovibrational states in the electronic states of HeT^+ we had to solve the rovibrational Schrodinger equation

$$\frac{d^2 f}{dR^2} + 2\mu [E - U_{nj}(R)] f(R) = 0 \quad (3)$$

where $U_{nj}(R)$ denotes the potential governing the nuclear motion and μ is the reduced mass of the nuclei. Equation (3) is obtained if the adiabatic, i.e. factorized form of the molecular wavefunction is assumed

$$\Psi = \Psi_n(\vec{r}_1, \vec{r}_2; R) f_{nvj}(R) R^{-1} Y_{jm}(\theta, \phi) \quad (4)$$

In the above wavefunction $\Psi_n(\vec{r}_1, \vec{r}_2; R)$ denotes the electronic wavefunction computed for the fixed internuclear distance R , $Y_{jm}(\theta, \phi)$ is the rotational wavefunction and $f_{nvj}(R)$ describes the vibrational motion. The dependence of the vibrational wavefunction on the rotational quantum number j arises from the centrifugal term in the nuclear motion potential U_{nj} appearing in Eq.(3). This potential has the form

$$U_{nj}(R) = \frac{j(j+1)}{2\mu R^2} + U_n^{BO}(R) + U_n^{ad}(R) + U_n^{rel}(R) \quad (5)$$

where $U_n^{BO}(R)$ denotes the Born-Oppenheimer (or clamped nuclei) potential for the n -th electronic state, obtained by solving the electronic Schrodinger equation, $U_n^{ad}(R)$ is the diagonal correction for nuclear motion, and $U_n^{rel}(R)$ is the relativistic correction to the potential which is small and has been included only for T_2 .

If the direction of the emitted β -electron does not coincide with the direction of the molecular axis, rotation of the molecule is excited. This rotation gives rise to the centrifugal potential barrier in the potential, leading to rotational dissociation from the quasibound vibrational and scattering states whose energies are above the dissociation limit. In the electronic ground state of HeT^+ there are 300 stable rovibrational states. Transition probabilities to all rovibrational states and to the region of the continuum spectrum have been computed and the resulting probability histogram is shown in Fig.2. The ground state dissociation limit is at $E = 0$. Thus transitions to the $E > 0$ region include transitions to the quasibound and continuum states. It follows from the histogram that they

occur with a probability of 16.57%, which is only smaller by a factor of 2.5 than the transition probability to the bound rovibrational states, the latter amounting to 40.84%.

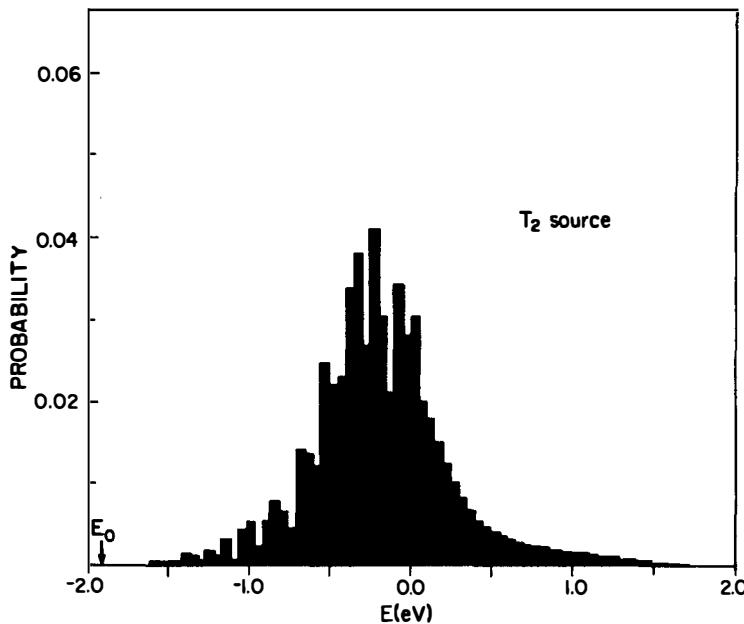


Fig.2. Probability histogram for transitions to the ground electronic state of s HeT^+ .

IV. Results and discussion

The best probability distribution, computed as described in the previous section, has been used to calculate the Kurie plots³. In Fig.3 we show some Kurie plots obtained for $m_{\nu} = 30$ eV using various models of the decaying system. The curves labeled "nuclear" and "atomic" show the results obtained for bare triton and for the T atom, respectively. The remaining results are for molecular T_2 . The $T_2(R = 1.4)$ curve shows results computed for the equilibrium internuclear distance $R = 1.4$ bohr. The "R-averaged" results which on the graph are indistinguishable from the previous one, have been obtained by averaging the electronic transitions over the zero-point vibrations in the initial state of T_2 . The " T_2 (final)" curve has been computed taking explicitly into account all transitions to

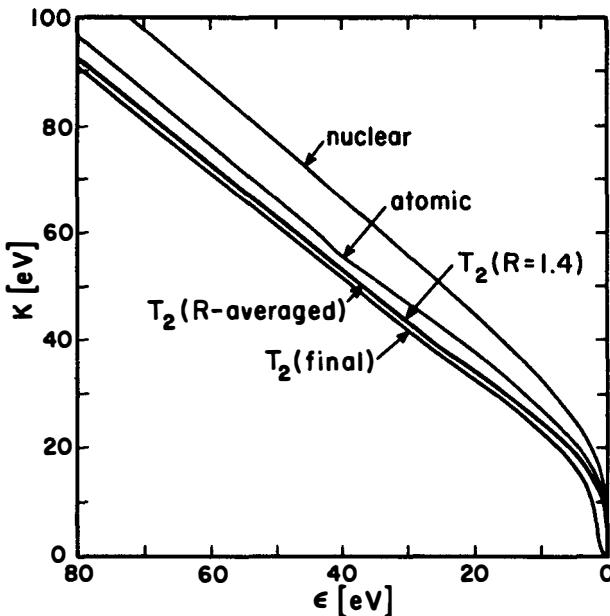


Fig. 3. Comparison of pure nuclear, atomic, and molecular T_2 Kurie plots for tritium β decay and for $m_{\nu} = 30$ eV.

rovibrational and continuum states in the lowest electronic states of ${}^3\text{HeT}^+$. These transitions considerably change the Kurie plot near the end point, and may have a large effect on the determined value of the neutrino mass if the latter is small, i.e. of the order of 1 eV or less.

We have also studied the effect of various models of tritium β -decay and of the experimental resolution on the determined value of the neutrino mass. The following procedure was employed: We have used our best probability function, assumed $m_\nu = 30$ eV or $m_\nu = 1$ eV, and the spectrum thus obtained was convoluted with two different resolution functions. Next we generated the "experimental" spectrum by the Monte Carlo method, fitted the spectrum with various models, and for each model we determined m_ν .

The results are shown in Table 1. It is seen that they are sensitive to the resolution function, and if $m_\nu = 30$ eV one can expect that any reasonable molecular model would give fairly reliable results. The entry GTO CI in Table 1 corresponds to a configuration interaction type wavefunction in which Gaussian type orbitals have been used¹². This wavefunction gives considerably worse energies for HeT^+ as compared with our values but, in spite of that, it would lead to a fairly accurate value of m_ν . This situation changes considerably for $m_\nu = 1$ eV. In this case very accurate results are needed to derive an m_ν value with, say, 50% accuracy. One may expect that if m_ν equals a few eV the situation will be less optimistic than for $m_\nu = 30$ eV, and fairly accurate Kurie plots will be needed for a reliable determination of m_ν .

The results presented above refer to molecular T_2 . The question arises, how big are the solid state effects that will have to be taken into account to extract the m_ν value from the LLNL frozen tritium experiment. Five such effects can be considered:

1. The fractional change of the T_2 wavefunction, $\Delta\Psi/\Psi$, caused by the binding in the crystal lattice. This is a small effect and amounts to $< 0.1\%$ in the wavefunction.
2. Perturbation due to the interaction of the HeT^+ ion (treated as a point charge) with the induced dipoles of the surrounding T_2 molecules results in less than an 0.8 eV shift of all excitation energies. In the lowest approximation this energy is independent of the HeT^+ state, and in such a case it affects only the end-point energy but not the value of m_ν . Since in a higher approximation the interaction depends on the state of HeT^+ , it has some effect on m_ν but being of a higher order this effect can be expected to be small.

Table 1. Effect of various model spectra on neutrino mass

| Resolution Function | | | | |
|---------------------------|--|---------------------------|---------|----------------|
| | ITEP 1984 Forward half width 22 eV | Gaussian FWHM = 4.7 eV | | |
| | m_ν | Δm_ν | m_ν | Δm_ν |
| Reference $m_\nu = 30$ eV | | | | |
| Bare nucleus | 6.4 | 24 | 12.3 | 18 |
| Two-level atomic | 25.5 | 5 | 25.4 | 5 |
| Atomic | 25.2 | 5 | 25.3 | 5 |
| GTO CI, R = 1.4 bohr | 29.2 | <1 | 29.3 | <1 |
| This work r = 1.4 bohr | 30.0 | <1 | 30.0 | <1 |
| " " R-averaged | 30.2 | <1 | 30.3 | <1 |
| " " final | 29.9 | <1 | 30.2 | <1 |
| Reference $m_\nu = 1$ eV | | | | |
| Bare nucleus | * 0.00 | 1 | | |
| Atomic | 0.00 | 1 | | |
| GTO CI, R = 1.4 bohr | 0.00 | 1 | | |
| This work R = 1.4 bohr | 0.42 | ≤ 1 | | |
| " " R-averaged | 1.92 | ≤ 1 | | |
| " " final | 1.00 | ≤ 1 | | |

3. Recoilless β -decay ("Mossbauer effect") has been found to be completely negligible⁶.

4. The sudden charge change of the decaying nucleus may induce excitations not only of the daughter ion but also of the surrounding T_2 molecules. This effect is expected to be small and will be computed in the near future.

5. Multiple scattering of the β -electron by surrounding T_2 molecules. This effect will be computed in the near future using the methods developed earlier¹⁴. It may be added that the multiple scattering effect is source thickness dependent and its magnitude can be studied experimentally by varying the thickness of the T_2 layer.

V. Conclusions

1. If m_ν is about 30 eV or larger a considerably less sophisticated approach than that presented above is sufficient to extract a reliable m_ν value from the experimental data.
2. If m_ν is less than about 1 eV, and the experimental resolution reaches this high degree of accuracy, both the theory and its numerical implementation must be improved.
3. In any case, we can say that results have been obtained needed for a neutrino mass determination with an error not exceeding a few tenths of an eV.

This work was supported under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No.W-7405-ENG. It was also supported in part by National Science Foundation Grant No. CHE-82007220, Division of Sponsored Research of the University of Florida, and Polish Academy of Sciences Grant MR.I.9.

References

1. W.Kolos, B.Jeziorski, K.Szalewicz and H.J.Monkhorst, Phys. Rev. A 31, 551 (1985).
2. B.Jeziorski, W.Kolos, K.Szalewicz, O.Fackler and H.J.Monkhorst, Phys. Rev. A 32, 2573 (1985).
3. O.Fackler, B.Jeziorski, W.Kolos, H.J.Monkhorst and K.Szalewicz, Phys. Rev. Lett. 55, 1388 (1985).
4. W.Kolos, B.Jeziorski, H.J.Monkhorst and K.Szalewicz, Intern. J. Quantum Chem. S 19, 000 (1985).
5. O.Fackler, B.Jeziorski, W.Kolos, H.J.Monkhorst and K.Szalewicz, to be published.
6. F.N.D.Kurie, J.R.Richardson and H.C.Paxton, Phys. Rev. 49, 368 (1936).
7. R.D.Williams and S.E.Koonin, Phys. Rev. C 27, 1815 (1983).
8. L.Wolniewicz, J.Chem.Phys. 78, 6173 (1983).
9. W.Kolos and L.Wolniewicz, J.Chem.Phys. 41, 3663 (1964).
10. W.Kolos and L.Wolniewicz, J.Mol.Spectrosc. 54, 303 (1975).
11. H.S.Taylor, G.V.Nazaroff and A.Golebiewski, J.Chem.Phys. 45, 2872 (1966); H.S.Taylor, Adv.Chem.Phys. 18, 91 (1970).
12. O.Fackler and N.Winter, Unpublished; O.Fackler, M.Mugge, H.Sticker, N.Winter and R. Woerner, Proceedings of the Fourth Moriond Workshop on Massive Neutrinos in Astrophysics and Particle Physics, La Plagne, Savoie, France 1984, edited by J.Tran Thanh Van (Edition Frontiers, Paris), p.273.
13. L.Z.Stolarczuk and H.J.Monkhorst, unpublished.
14. W.Kolos, H.J.Monkhorst and K.Szalewicz, J.Chem.Phys. 77, 1323, 1335 (1982); K.Szalewicz, W. Kolos, H.J.Monkhorst and C.Jackson, J.Chem.Phys. 80, 1435 (1984).