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and Their Effect on a Precision Neutrino
Mass Experiment

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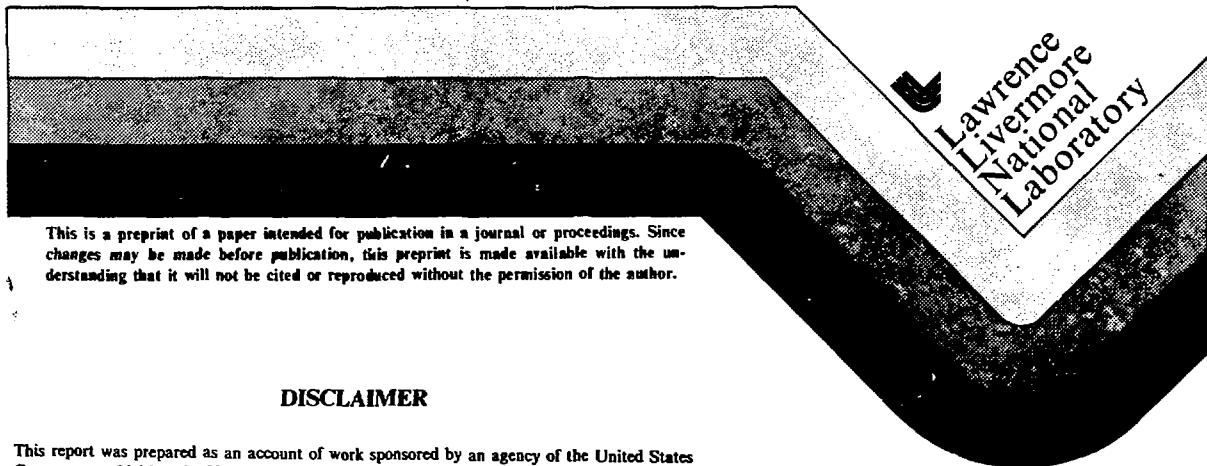H. Sticker
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THE CALCULATION OF MOLECULAR FINAL STATES
AND THEIR EFFECT ON A PRECISION NEUTRINO MASS EXPERIMENT* .

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ABSTRACT

We are performing an experiment to determine the electron neutrino
mass with the precision of a few electron volts by measuring the tritium
beta decay energy distribution near the endpoint. At the few electron
volt level, a major consideration in the choice of a tritium source is the
effect of excited final atomic or molecular states on the beta decay
distribution. It is important to choose a source for which the initial
and final states can be accurately calculated. We have chosen frozen
tritium as our source since the states of molecular tritium and those of
the HeT^+ daughter ion have electronic wavefunctions that can be calculated
with high accuracy. We describe the effects of final excited states on
the neutrino mass determination and the results of these calculations in
this paper.

The choice of a source for our tritium bet- decay experiment
(described in an accompanying paper) is extremely important. Several
problems need to be addressed in choosing the best source. The first is
that if the neutrino mass is zero, the fraction of decays within 2 eV of
the endpoint is only 2.6×10^{-12}. This small fraction necessitates a source
of high activity, but one that is thin in order to keep the dE/dx loss of
the emerging beta small. Even if the neutrino has a small finite mass,
the major distortion of the spectrum occurs within a few neutrino masses
from the endpoint.
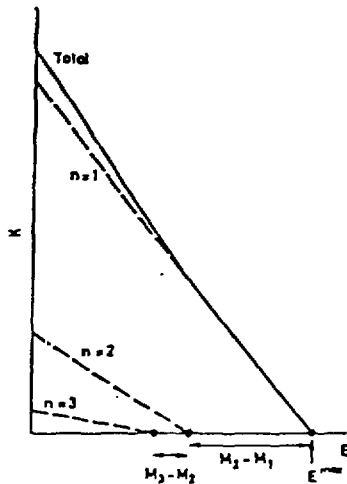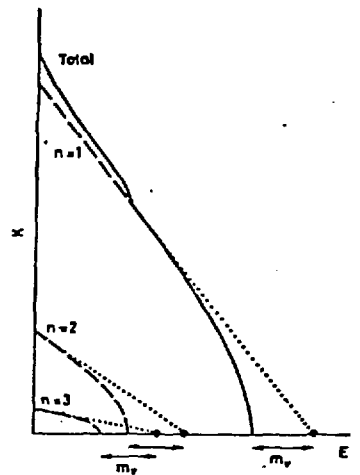
Fig. 1a   Fig. 1b

The second problem is that the decaying atom or molecule remains in one
of many excited states. These excited states degrade the beta energy and
give rise to a number of branches in the tritium beta decay spectrum each
with different endpoint energies. The sum of these branches gives rise to
the distorted measured spectrum. The effect of these different excited
final states on the Kurie plot for a zero mass neutrino is shown in Fig.
1a and for a finite mass neutrino in Fig. 1b. These figures show that a
precision neutrino mass experiment must accurately account for these final
states. Unfortunately the transition probabilities and energy levels of
the final states are not calculable with sufficient precision for most

complex molecules or tritium binding processes which might serve as sources.

These two considerations, along with others, led us to chose pure molecular tritium (T_2) frozen at liquid helium temperatures as our source.

This source is ideal because it has:

1) a very high specific activity -- the highest possible for a given dE/dx loss, and

2) a very low intermolecular binding energy (on the order of 1/400 eV), which means that the electronic wavefunction is essentially that of the free T_2 molecule.

We have done the final state calculations for free molecular tritium although the actual source is frozen tritium. Nevertheless, the tritium molecular wavefunction in the frozen solid is very close to the molecular wavefunction of the free molecule. We can understand this fact qualitatively by noting that the tritium melting temperature implies that the intermolecular binding energy is very much less than the orbital electron binding energy. Consequently we can expect a very small perturbation on the molecular wavefunction because of intermolecular binding forces.

More quantitively, the electron probability density at the half nearest molecular neighbor distance is approximately 3×10^{-4} of the maximum. This small electronic overlap gives rise to a negligible distortion of the molecular wavefunction. The depth of the internuclear potential well is approximately 1,600 times deeper than the intermolecular potential well. This difference in binding energies also indicates a very small perturbation of the molecular wavefunction in the solid.

A theoretical calculation of the change in the T_2 electronic wavefunction resulting from the effects of binding tritium in the crystal lattice was done by L. Stolarzik, Warsaw (Reported to us by H. Monkhorst, University of Florida). He symmetrically orthogonalized the wavefunctions and found that the fractional change in the wavefunction, $\Delta\psi/\psi$, is approximately 0.07%. This small change is not surprising since the inductive forces which bind the tritium molecules in the solid are

typically one to two orders of magnitude smaller than the exchange forces which govern molecular binding.

The experimental evidence for a very small change in the electronic wavefunction resulting from the binding in the solid comes from Raman spectra in gaseous and solid hydrogen. The vibrational energy levels are determined by the shape of the internuclear potential well and the shape of this well is determined by the electronic wavefunction. The typical measured shift in the vibrational energy levels resulting from the binding in solid hydrogen is about 1/2000 eV. Since this energy shift is very small compared with the typical vibrational energy level spacing of about 0.1 eV, this is evidence for a very small perturbation in the molecular wavefunctions resulting from the intermolecular binding in the solid. Furthermore, the molecular binding forces are so weak that the rotational states are hardly perturbed and the molecules can rotate as though they were nearly free.

Hence, conservatively, we can conclude that the uncertainty in the transition probabilities due to intermolecular binding in the solid is less than 0.5% and much smaller for the energy level uncertainties.

Because this essentially free tritium molecule is a two electron system, the final molecular excited state effects can be accurately calculated. The probability for a molecular transition to occur upon beta decay is given by

$$P_{if} = \left| \int \psi_f^* T_{op} \psi_i d\tau \right|^2$$

where ψ_f and ψ_i are the final and initial state wavefunctions and T_{op} is the operator taking the initial state into the final state upon beta decay. With a high degree of accuracy, we can partially make the Born-Oppenheimer approximation and separate the molecular wavefunction into the electronic wavefunction, ϕ^{el}, and the nuclear wavefunction, $\chi_{v,j}^{nuc}$, which depends on both the vibrational quantum number, v, and the rotational quantum number, j.

$$\psi = \phi^{el} \chi^{nuc}_{\nu,j}$$

Since T_{op} does not depend on the electronic coordinates, the transition probability can then be rewritten as

$$P_{if} = |\int A_{if} \chi_f^* T_{op} \chi_i d\tau |^2$$

where

$$A_{if} = \int \phi_{el}^*(\vec{r}) \phi(\vec{r}) d\vec{r}.$$

The electronic wavefunctions are determined by a complete configuration interaction calculation. The internuclear potential energy for each of the excited states is calculated along with the electronic wavefunctions. The nuclear wavefunctions are determined for each of these electronic states by solving Schroedingers equation for that potential energy function. For the bound states, the nuclear wavefunctions are determined for each vibrational and rotational quantum number.

As will be discussed later, the initial state $\psi_i = \phi_i^{el} \chi^{nuc}_{\nu,j}$ for the T_2 molecule can be accurately taken as the ground electronic state and the $\nu = 0, j = 0$ nuclear motion state. On the other hand there will be a distribution of final states in each degree of freedom.

Figure 2 shows the final state potential energy curves for the HeT^+ daughter ion as a function of the helium-tritium internuclear distance for the first twenty eight states. Most of these molecular states have the wrong electronic configuration to have any appreciable transition probability. The transition probabilities for these states are shown as a function of the $He-T^+$ internuclear separation in Figure 3. This figure shows that at the initial T_2 internuclear separation, 1.4 A. U., there are only five electronic states, including the ground state, which have sufficiently large transition probabilities to give rise to distinct

branches in the Kurie plot. As is expected from the closeness of the T_2
and the HeT$^+$ ground state internuclear separations, most of the
probability occurs for a transition to the HeT$^+$ ground state. The
probability of finding the HeT$^+$ ion in the ground state after the decay is
approximately 60% which is to be compared with 70% in the decay of an
isolated tritium atom. Note that the calculations accurately reproduce
the atomic tritium transition probabilities for large internuclear
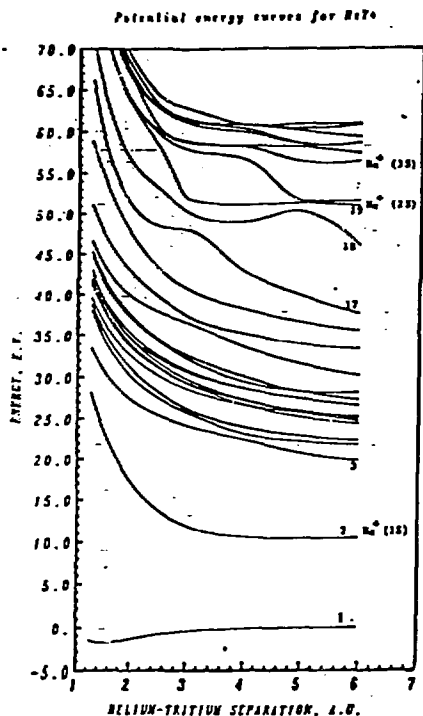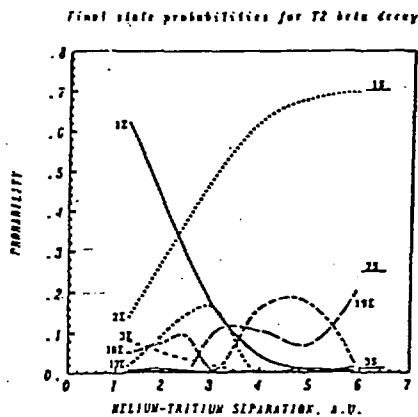separations.

Fig. 2

Fig. 3

Unlike the atom, however, the HeT$^+$ molecule in its ground state has
two additional degrees of freedom which can absorb energy from the decay
beta. These two additional degrees of freedom are the vibrational and
rotational states.

At the liquid helium temperature of our source, only the lowest
vibrational and the lowest rotational states are populated. However, after
the decay, when one of the atoms has been given an impulse from the decay
beta, most of the possible vibrational and rotational states will be
populated. Fortunately, even near the endpoint of the beta decay spectrum
where the maximum momentum transfer to the nucleus can occur, the energy
transferred to the nucleus is too small to dissociate the HeT$^+$ daughter
ion.

The HeT$^+$ is primarily excited to a high vibrational state when, near
the endpoint of the beta decay distribution, the decay beta is emitted
nearly aligned with the internuclear axis. Conversely, the HeT$^+$ ion is
left in a highly excited rotational state when the decay beta is emitted
nearly perpendicular to the internuclear axis. This coupling between the
beta decay and the vibrational and rotational states is shown in Fig. 4 as
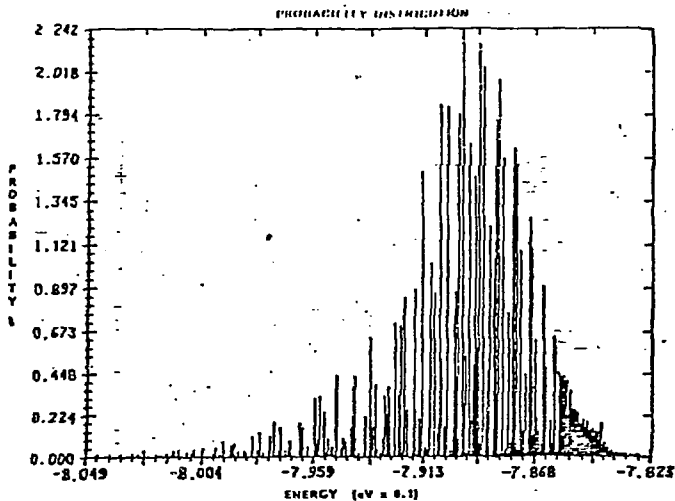a high density of states near the top of the potential well.

Fig. 4

The probability of finding the HeT$^+$ in in a particular vibrational
and rotational state versus the energy of these states are shown in Figure
4. The full width of this distribution is about 2 eV and the full width

at half height is on the order of 1 eV. As a consequence of this small spread, the ground state branch in the Kurie plot is smeared by only an average of 1 eV. This additional spread is a small penalty to pay for the ease of using molecular rather than atomic tritium.

Our conclusion is that frozen tritium is an ideal source because:

1) The molecular final state effects are well calculable and the uncertainties in these calculations due to calculational accuracy and intermolecular binding effects result in an uncertainty in the determination of the neutrino mass of less than 1 eV.

2) It is pure tritium and consequently it is the most intense source for a given dE/dx loss.

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