RADIATIVE TRANSITION PROBABILITY FROM THE (3/2+) STATE TO THE (3/2−) STATE IN He^5 NUCLEUS

by

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Submitted in partial fulfillment
of the requirements for the degree of
Master of Science

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ABSTRACT

The radiative transition probability from the (3/2+) state at 16.69 Mev. to the (3/2-) ground state in He^5 is calculated using cluster model wave functions. In this model, the second excited state is assumed to have a "t-d" cluster structure and the ground state an "α-n" cluster structure. A method of antisymmetrization of the wave functions not involving the isospin greatly simplifies the calculation of matrix elements.

The result is found to be in quite close agreement with the experimental value, thus confirming a high degree of accuracy of the cluster model wave functions for He^5.

ACKNOWLEDGEMENTS

The author wishes to thank Dr. R.C. Smith for suggesting the problem and for his advice throughout the work.

He is grateful to Dr. J.M. Robson for permission to use the X~~Z~~erox copier.

He also thanks Mr. Vo Ba Loc for his assistance in the preparation of the thesis and Mr. G.L. Cornish for his help in printing the thesis.

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CHAPTER I

INTRODUCTION

The cluster model has had some success in predicting the low-lying energy levels of some light nuclei (2, page 47)*. In particular, Pearlstein, Tang and Wildermuth (6) have attained relatively good results in calculating the energies of the first three levels in He^5 on the basis of the cluster model.

In this work, using the same model, we shall calculate the radiative transition probability from the second excited state (3/2 +) to the ground state (3/2 -) in He^5 (fig.1). Since a change in cluster configuration is expected in this transition, it seems reasonable that such a calculation would be a fairly sensitive test of the cluster model wave functions.

In the cluster model, there is some kind of correlation between the nucleons which is favoured in different nuclear states. Thus, the ground state (3/2 -) of He^5 is considered as composed of an alpha-particle cluster and a neutron.

The spatial wave function describing this state is:

$$(I-1) \qquad \varphi(\tfrac{3}{2}-) = \varphi(\alpha)\,\varphi(n)\,\chi(\vec{R}_\alpha - \vec{R}_n)\,W(R_{cm})$$

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* The number enclosed in parentheses refers to the references listed at the end of the thesis.

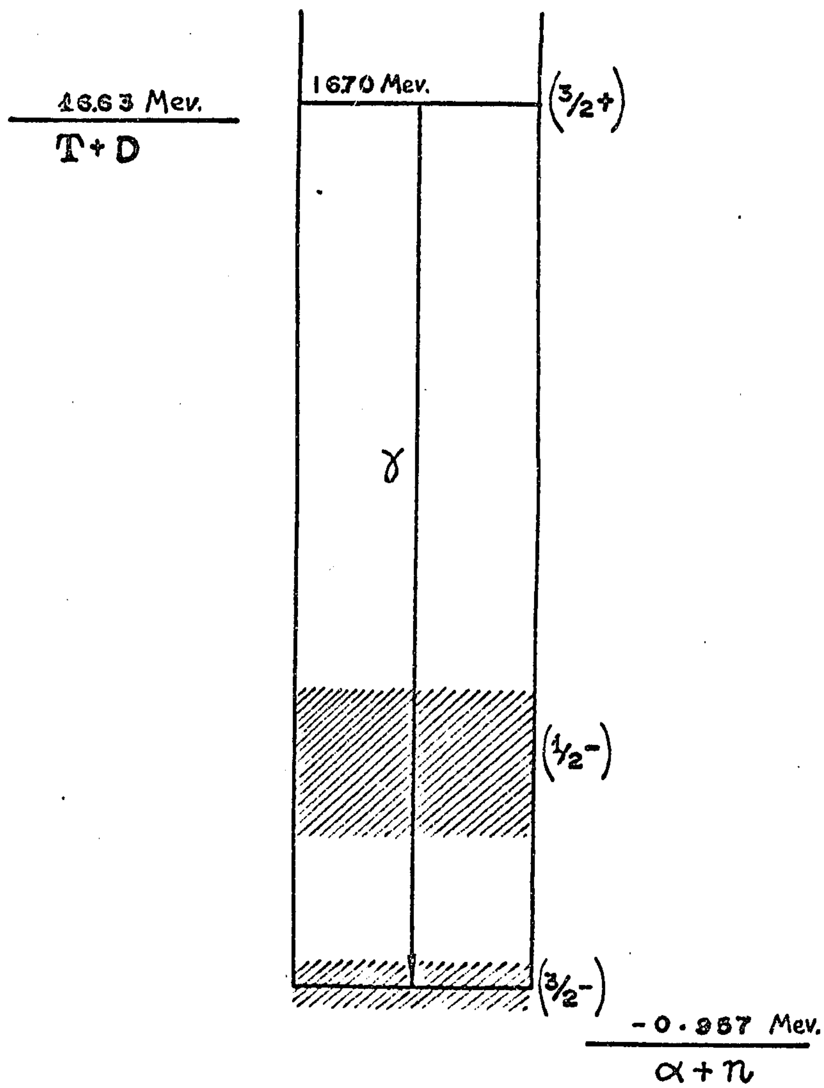

Fig.1 Energy level diagram for the He^5 nucleus. The proximity of the α-n and d-t reaction thresholds to the (3/2 -) and (3/2 +) levels respectively suggests that the (3/2 -) state has an "α-n" cluster structure and the (3/2 +) a "t-d" cluster structure.

The first two functions describe the internal motions of the two clusters, $\chi(\vec{R}_\alpha - \vec{R}_n)$ describes the relative motion of the two clusters, and the wave function of the center-of-mass $W(R_{cm})$ is included for mathematical convenience (it will be dropped later as we shall see in Chapter IV).

Explicitly, (I-1) can be written as:

$$(\text{I-2}) \qquad \varphi(\tfrac{3}{2}-) = \exp\left(-\frac{\alpha_1}{2}\sum_{i=1}^{4} r_i''^2\right) R_1^n \mathcal{Y}_\ell^m(\Omega_1) \exp\left(-\frac{2\beta'}{5} R_1^2\right) \exp\left(-\frac{5\gamma}{2} R_{cm}^2\right)$$

where:

$$\vec{r}_i'' = \vec{r}_i - \vec{R}_\alpha \qquad (i = 1,2,3,4)$$

$$\vec{R}_\alpha = \tfrac{1}{4}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4)$$

$$\vec{R}_1 = \vec{R}_\alpha - \vec{r}_5$$

$$\vec{R}_{cm} = 1/5\ (\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4 + \vec{r}_5)$$

In the independent particle model, all nucleons move in an oscillator potential; the ground state of He^5 must therefore have one quantum of energy $\hbar\omega$ (fig.2). In the cluster model, we assume that there is no internal excitation in the alpha cluster, so that the relative motion part $\chi(\vec{R}_\alpha - \vec{R}_n)$ is an oscillator function with one quantum of energy, that is:

$$N = 2(n-1) + \ell = 1$$

$$\text{or:} \quad n = \ell = 1$$

It is emphasized here that, in the generalized cluster model, the width parameters α_1, β' do not have the same value; their numerical values are determined by the Ritz variational method (6). In this method, $\langle H \rangle$ is evaluated as a function of the parameters α_1, β' and the minimum of

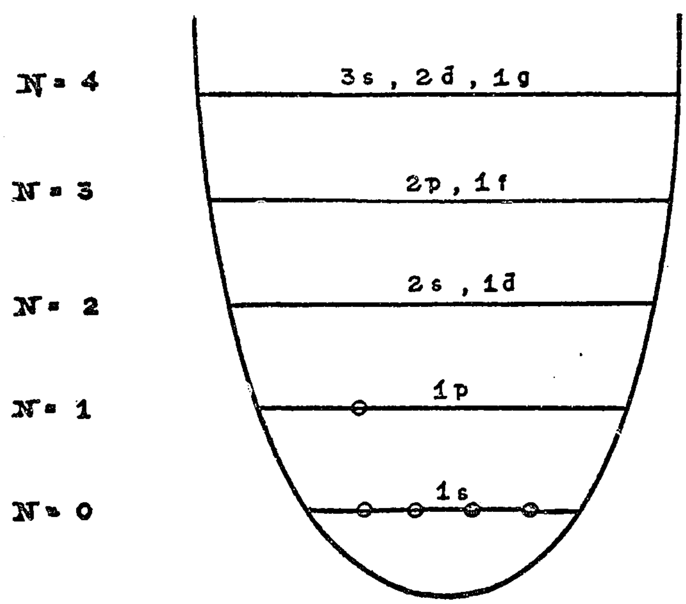

Fig. 2

o neutron

⊚ proton

In the independent particle model, the ground state has two neutrons and two protons in the 1s state of the oscillator potential and one neutron in the 1p state ; thus it has one quantum of energy $\hbar\omega$.

$\langle H \rangle$ is taken to correspond with the energy of the ground state.

The second excited state (3/2 +) cannot be described by this "α - n" configuration since it is a resonance level with a large lifetime and it can be shown that in this circumstance, $\langle H \rangle$ has no minimum with respect to variations in the above width parameters. Therefore, we take instead the configuration of triton plus deuteron to represent this state. It is found that the phenomenon of very narrow levels suddenly following above very broad levels in many nuclei in addition to He^5 can be characterized by such a change in structure (2, page 52). Moreover, the proximity of the d-t reaction threshold (at 16.63 Mev., see fig. 1) suggests that the cluster wave function, using the "triton-deuteron" configuration might be a reasonable approximation to the actual wave function for the (3/2 +) state.

The wave function describing the (3/2 +) state is then:

(I-3) $$\varphi(\tfrac{3}{2}+) = \varphi(t)\,\varphi(d)\,\chi(\vec{R}_t - \vec{R}_d)\,W(R_{cm})$$

$$= \exp\left(-\frac{\alpha}{2}\sum_{i=1}^{3} r_i'^2 - \frac{\bar{\alpha}}{2}\sum_{j=4}^{5} r_j'^2\right) R^n\, \mathcal{Y}_\ell^m(\Omega)\, \exp\left(-\frac{3\beta}{5}R^2\right)$$

$$\times \exp\left(-\frac{5\gamma}{2}R_{cm}^2\right)$$

where: $\vec{r}_i' = \vec{r}_i - \vec{R}_t \qquad (i = 1,2,3)$

$\vec{r}_j' = \vec{r}_j - \vec{R}_d \qquad (j = 4,5)$

$\vec{R}_t = 1/3\ (\vec{r}_1 + \vec{r}_2 + \vec{r}_3) \quad ; \quad \vec{R}_d = \tfrac{1}{2}\ (\vec{r}_4 + \vec{r}_5)$

$\vec{R} = \vec{R}_t - \vec{R}_d$

Here again, the triton and deuteron clusters are in their ground states (no internal excitations), and for the relative motion of the two clusters, we use $n = 2$ and $l = 0$ to get two quanta of energy for this excited state (3/2 +).

*

* *

Chapter II will be devoted to the antisymmetrization of the initial state (3/2 +) and the final state (3/2 -) wave functions of the He^5 nucleus.

In Chapter III, a mathematical derivation of the radiative transition probability T_{if} is carried out; it is assumed there that only the electric dipole matrix element is responsible for the transition. T_{if} is found to depend on one type of integral which we call I_k. This integral will be evaluated in Chapter IV.

Chapter V will be devoted to the numerical calculation of T_{if} and thence of the level width Γ_γ for gamma emission. This theoretical value of Γ_γ will be compared with the experimental results found by different authors.

CHAPTER II

ANTISYMMETRIZATION OF THE "CLUSTER MODEL" WAVE FUNCTIONS.

In order to calculate the matrix element of the electric dipole operator $\langle Af|Q_{1\mu}|Ai\rangle$, where Af and Ai are the antisymmetrized wave functions of the final and initial states respectively, we must first antisymmetrize these wave functions.

Some useful notations are defined to facilitate the antisymmetrization.

The spatial part of the 'cluster model' wave functions for the initial and final states of the He^5 nucleus will be written respectively as follows :

(123;45) and (1234;5)

The first two positions and fifth position denote the neutrons, the third and fourth positions denote the two protons; the numbers denote different particles. Thus 1, 2 and 5 are neutrons and 3, 4 are protons in the preceding notations. The semi-colons in these expressions indicate the fact that the initial state has a triton and a deuteron cluster while the final state has an alpha-particle cluster plus one neutron.

Our method of antisymmetrization of the wave functions differs from that of Wildermuth and Kanellopoulos (3) in that we antisymmetrize the protons and the neutrons separately. In other words, the protons and the neutrons are not considered as identical particles. This method of antisymmetrization has been proved to be equivalent to that in which the isotopic spin is introduced when calculating matrix elements of operators not involving isotopic spin (4).

This method has two advantages: first, isospin need not be included in the wave functions, and second, for the case in which the operator $Q_{1\mu}$ is symmetric only w... res- pect to protons and neutrons separately as occurs here, the calculation of its matrix element will be greatly simplified. This second point will become apparent in Chapter III.

1.- Antisymmetrization operator.-

The antisymmetrization operator can be written as (4):

(II-1) $$A = A_n A_p$$

where A_n and A_p are respectively the antisymmetrization operators for the neutrons 1, 2, 5 and for the protons 3, 4 :

(II-2) $$A_n = \frac{1}{3!} \sum_n (-)^{\pi_n} \Pi_n \quad ; \quad A_p = \frac{1}{2!} \sum_p (-)^{\pi_p} \Pi_p$$

Π_n and Π_p are the permutation operators which act on the neutrons and protons respectively.

The antisymmetrized "cluster model" wave functions are then:

(II-3) $$\Phi_i = N_i A \varphi_i = N_i A \left\{ (123;45) \chi_i \right\}$$

(II-4) $$\Phi_f = N_f A \varphi_f = N_f A \left\{ (1234;5) \chi_f \right\}$$

where χ_i and χ_f are the spin wave functions of the initial and final states respectively .

Here, we make a distinction between the eigenfunctions φ_i , φ_f of the initial and final states and the antisymmetrized wave functions of these states Φ_i and Φ_f . N_i and N_f are the normalization factors which can be calculated from:

(II-5) $$\langle \Phi_i | \Phi_i \rangle = N_i^2 \langle A\varphi_i | A\varphi_i \rangle = 1$$

(II-6) $$\langle \Phi_f | \Phi_f \rangle = N_f^2 \langle A\varphi_f | A\varphi_f \rangle = 1$$

2.- Antisymmetrization of the initial state wave function.-

$$\Phi_i = N_i A \left\{ (123;45) \chi_i \right\}$$

We must first write the spin eigenfunction χ_i of the initial state. In this state, The He^5 nucleus is composed of a triton and a deuteron cluster. The spin wave function of the nucleus must therefore be formed from the spin wave functions of the triton and the deuteron. The triton has $J^\pi = \frac{1}{2}^+$, while for the deuteron, $J^\pi = 1^+$.

Thus, if $|SM\rangle$ is the spin wave function of the He^5 nucleus, and $|s_1 m_1\rangle$ and $|s_2 m_2\rangle$ are respectively the spin wave functions of the triton and deuteron clusters, then :

(II-7) $$|SM\rangle = \sum_{m_1+m_2=M} |s_1 m_1\rangle |s_2 m_2\rangle \langle s_1 s_2 m_1 m_2 | SM\rangle$$

The "triton-deuteron" is a $J = 3/2$ state having $L = 0$ for the relative motion of the two clusters; hence:

$$\vec{S} = \vec{J} - \vec{L} \quad \text{so that} \quad \vec{S} = \vec{J}$$

and therefore : $S = 3/2$

From (II-7) we deduce:

$$
\text{(II-8)}\quad
\begin{cases}
\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle = \left|\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle_t \left|1\,1\right\rangle_d \\
\left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle = \left(\tfrac{2}{3}\right)^{\frac{1}{2}} \left|\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle_t \left|1\,0\right\rangle_d + \left(\tfrac{1}{3}\right)^{\frac{1}{2}} \left|\tfrac{1}{2}\,-\tfrac{1}{2}\right\rangle_t \left|1\,1\right\rangle_d \\
\left|\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle = \left(\tfrac{2}{3}\right)^{\frac{1}{2}} \left|\tfrac{1}{2}\,-\tfrac{1}{2}\right\rangle_t \left|1\,0\right\rangle_d + \left(\tfrac{1}{3}\right)^{\frac{1}{2}} \left|\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle_t \left|1\,-1\right\rangle_d \\
\left|\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle = \left|\tfrac{1}{2}\,-\tfrac{1}{2}\right\rangle_t \left|1\,-1\right\rangle_d
\end{cases}
$$

The ground state of the deuteron is a triplet state, so that its spin wave functions are:

$$
\text{(II-9)}\quad
\begin{cases}
\left|1\,1\right\rangle_d = \alpha_4 \alpha_5 \\
\left|1\,0\right\rangle_d = \frac{1}{\sqrt{2}} \left(\alpha_4 \beta_5 + \beta_4 \alpha_5\right) \\
\left|1\,-1\right\rangle_d = \beta_4 \beta_5
\end{cases}
$$

where α_k indicates that particle k is in a state having $m_s = \frac{1}{2}$, while β_k indicates that particle k is in a state having $m_s = -\frac{1}{2}$.

For the triton, the choice of the spin wave function is much more complicated. This choice is not unique for we have here a problem of addition of three angular momenta.

We know that the spin of the triton in the ground state is $\frac{1}{2}$ (9, page 193); this can be formed in several different ways. The spins of nucleons 1 and 2 (2 neutrons) can first be coupled: $\vec{s}_1 + \vec{s}_2 = \vec{s}_{12}$, and then this resulting spin coupled to $\vec{s}_3$ (spin of the proton) : $\vec{s}_{12} + \vec{s}_3 = \vec{S}$ to give the total spin $S = \frac{1}{2}$.

Since the coupling of the two spins gives two possible values 0 and 1 to s_{12} , this gives rise to two different sets of spin wave functions for the triton:

(1).- $s_{12} = 0$

$$\text{(II-10)} \quad \begin{cases} \left|\frac{1}{2}\,\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{2}} \; (\alpha_1\beta_2 - \beta_1\alpha_2)\,\alpha_3 \\ \left|\frac{1}{2}\,-\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{2}} \; (\alpha_1\beta_2 - \beta_1\alpha_2)\,\beta_3 \end{cases}$$

(2).- $s_{12} = 1$

$$\text{(II-11)} \quad \begin{cases} \left|\frac{1}{2}\,\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{6}} \left[(\alpha_1\beta_2 + \beta_1\alpha_2)\,\alpha_3 - 2\,\alpha_1\,\alpha_2\,\beta_3 \right] \\ \left|\frac{1}{2}\,-\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{6}} \left[(\alpha_1\beta_2 + \beta_1\alpha_2)\,\beta_3 - 2\,\beta_1\,\beta_2\,\alpha_3 \right] \end{cases}$$

A different scheme is to couple first the spins of nucleons 1 and 3 (a neutron and a proton) : $\vec{s}_1 + \vec{s}_3 = \vec{s}_{13}$ and then $\vec{s}_{13}$ and $\vec{s}_2$: $\vec{s}_{13} + \vec{s}_2 = \vec{S}$. This is equivalent to permuting 2 and 3 in the two sets of spin wave functions (II-10) and (II-11) :

(3).- $s_{13} = 0$

$$\text{(II-12)} \quad \begin{cases} \left|\frac{1}{2}\,\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{2}} \; (\alpha_1\beta_3 - \beta_1\alpha_3)\,\alpha_2 \\ \left|\frac{1}{2}\,-\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{2}} \; (\alpha_1\beta_3 - \beta_1\alpha_3)\,\beta_2 \end{cases}$$

(4).- $s_{13} = 1$

$$\text{(II-13)} \quad \begin{cases} \left|\frac{1}{2}\,\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{6}} \left[(\alpha_1\beta_3 + \beta_1\alpha_3)\,\alpha_2 - 2\alpha_1\beta_2\alpha_3 \right] \\ \left|\frac{1}{2}\,-\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{6}} \left[(\alpha_1\beta_3 + \beta_1\alpha_3)\,\beta_2 - 2\beta_1\alpha_2\beta_3 \right] \end{cases}$$

A third alternative is to couple first $\vec{s}_2$ and $\vec{s}_3$ and then $\vec{s}_{23}$ and $\vec{s}_1$, but the result is the same as the second scheme, since in these two schemes, we add first the spins of one neutron and one proton (nucleons 1,3 and nucleons 2,3) and then the spin of the remaining neutron to the resulting spin.

Of these four possible sets of spin wave functions for the triton, the second set must obviously be ruled out since it violates the Pauli principle: the spin wave function is symmetric with respect to the two neutrons 1 and 2 and so is the spatial wave function, so that when φ_i is antisymmetrized: $A\varphi_i = 0$.

We have tried the first and third sets of spin wave functions in the calculation of the matrix elements $\langle Af|Q_{1\mu}|Ai\rangle$ and we found that the matrix elements of the principal term of $Q_{1\mu}$ are zero(*); this is due to the symmetry character of these spin and spatial wave functions.

Therefore, we shall choose now the fourth set of spin wave functions (equation II-13), which are the only wave functions which do not make $\langle Af|\sum e_i r_i Y_1^{\mu *}|Ai\rangle = 0$

(*) The electric dipole operator $Q_{1\mu}$ is composed of two terms: $Q_{1\mu} = \sum_i e_i r_i Y_i^{\mu *}(\omega_i) - \frac{i\mu_0 k}{2} \sum_i g_{si}\, \vec{\sigma}_i \times \vec{r}_i \cdot \nabla(r Y_i^{\mu *})_i$

The second term is usually neglected because of its small contribution to the matrix elements compared to that of the first term, which is the principal term of $Q_{1\mu}$.

Substituting (II-9) and (II-13) in (II-8) gives the result:

$$
\text{(II-14)}\quad
\begin{cases}
\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle = \frac{1}{\sqrt{6}}\left[(\alpha_1\beta_3+\beta_1\alpha_3)\alpha_2 - 2\alpha_1\beta_2\alpha_3\right]\alpha_4\alpha_5 \\
\left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle = \frac{1}{\sqrt{18}}\left[(\alpha_1\beta_3+\beta_1\alpha_3)(\alpha_2\alpha_4\beta_5+\alpha_2\beta_4\alpha_5+\beta_2\alpha_4\alpha_5)\right. \\
\qquad\qquad \left. -2\alpha_1\beta_2\alpha_3(\alpha_4\beta_5+\beta_4\alpha_5) - 2\beta_1\alpha_2\beta_3\alpha_4\alpha_5\right] \\
\left|\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle = \frac{1}{\sqrt{18}}\left[(\alpha_1\beta_3+\beta_1\alpha_3)(\alpha_2\beta_4\beta_5+\beta_2\alpha_4\beta_5+\beta_2\beta_4\alpha_5)\right. \\
\qquad\qquad \left. -2\beta_1\alpha_2\beta_3(\alpha_4\beta_5+\beta_4\alpha_5) - 2\alpha_1\beta_2\alpha_3\beta_4\beta_5\right] \\
\left|\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle = \frac{1}{\sqrt{6}}\left[(\alpha_1\beta_3+\beta_1\alpha_3)\beta_2 - 2\beta_1\alpha_2\beta_3\right]\beta_4\beta_5
\end{cases}
$$

With these spin wave functions, the antisymmetrization results from a straightforward application of the operator $A = A_n A_p$ to the wave function $(123;45)\chi_i$.

As we shall see later, only the antisymmetrized wave function with $\chi_i = \left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle$ is needed (in the calculation of the normalization factor N_i) and it is given below:

$$
\begin{aligned}
\Phi_i\left(\tfrac{3}{2}\right) &= N_i \; A\left\{(123;45)\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle\right\} \\
\text{(II-15)}\qquad &= \frac{N_i}{4\sqrt{6}}\Big\{(\alpha_2\beta_1-\beta_2\alpha_1)\,\alpha_3\alpha_4\alpha_5\left[(123;45)-(124;35)\right] \\
&\quad +(\beta_2\alpha_5-\alpha_2\beta_5)\,\alpha_1\alpha_3\alpha_4\left[(523;41)-(524;31)\right] \\
&\quad +(\beta_5\alpha_1-\alpha_5\beta_1)\,\alpha_2\alpha_3\alpha_4\left[(153;42)-(154;32)\right]\Big\}
\end{aligned}
$$

3.- <u>Antisymmetrization of the final state wave function</u>.

In the final state, the total spin of the nucleus is $S = \frac{1}{2}$, since it is formed by the coupling of the spin of the alpha-particle (which is 0) and the spin of the single neutron.

As we have seen in Chapter I, the ground state of the He^5 nucleus has an angular momentum $L = 1$ for the relative motion of the two clusters, and its total angular momentum is $J = \frac{3}{2}$. Hence, the spin $S = \frac{1}{2}$ must be coupled to the angular momentum $L = 1$ to give the total angular momentum of the nucleus $J = \frac{3}{2}$:

$$|JM\rangle = \sum_{M_L + M_S = M} |SM_S\rangle\, |LM_L\rangle\, \langle SLM_S M_L | JM\rangle$$

Thus:

$$\text{(II-16)}\quad \begin{cases} \left|\frac{3}{2}\,\frac{3}{2}\right\rangle = |1\,1\rangle \left|\frac{1}{2}\,\frac{1}{2}\right\rangle \\ \left|\frac{3}{2}\,\frac{1}{2}\right\rangle = \left(\frac{1}{3}\right)^{\frac{1}{2}} |1\,1\rangle \left|\frac{1}{2}\,-\frac{1}{2}\right\rangle + \left(\frac{2}{3}\right)^{\frac{1}{2}} |1\,0\rangle \left|\frac{1}{2}\,\frac{1}{2}\right\rangle \\ \left|\frac{3}{2}\,-\frac{1}{2}\right\rangle = \left(\frac{2}{3}\right)^{\frac{1}{2}} |1\,0\rangle \left|\frac{1}{2}\,-\frac{1}{2}\right\rangle + \left(\frac{1}{3}\right)^{\frac{1}{2}} |1\,-1\rangle \left|\frac{1}{2}\,\frac{1}{2}\right\rangle \\ \left|\frac{3}{2}\,-\frac{3}{2}\right\rangle = |1\,-1\rangle \left|\frac{1}{2}\,-\frac{1}{2}\right\rangle \end{cases}$$

where: $\left|\frac{1}{2}\frac{1}{2}\right\rangle = \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5$

$\left|\frac{1}{2}\,-\frac{1}{2}\right\rangle = \alpha_1 \beta_2 \alpha_3 \beta_4 \beta_5$

and: $|1\, M_L\rangle = Y_1^{M_L}(\Omega)$

$Y_1^{M_L}(\Omega)$ is the angular part of the wave function of the relative motion and is simply a spherical harmonic with $L = 1$.

In order to obtain the complete wave function, all functions in (II-16) must be multiplied by internal wave functions (wave functions of the internal motion in the clusters) as well as by the radial part of the wave function associated with the relative motion.

Hence, from (II-16) the overall wave functions can be written explicitly as follows:

$$
\text{(II-17)} \quad \left\{ \begin{aligned}
\varphi_f(\tfrac{3}{2}) &= (1234;5)_{M_L=1}\, \alpha_1\beta_2\alpha_3\beta_4\alpha_5 \\
\varphi_f(\tfrac{1}{2}) &= (\tfrac{1}{3})^{\frac{1}{2}}(1234;5)_{M_L=1}\alpha_1\beta_2\alpha_3\beta_4\beta_5 + (\tfrac{2}{3})^{\frac{1}{2}}(1234;5)_{M_L=0}\alpha_1\beta_2\alpha_3\beta_4\alpha_5 \\
\varphi_f(-\tfrac{1}{2}) &= (\tfrac{2}{3})^{\frac{1}{2}}(1234;5)_{M_L=0}\alpha_1\beta_2\alpha_3\beta_4\beta_5 + (\tfrac{1}{3})^{\frac{1}{2}}(1234;5)_{M_L=-1}\alpha_1\beta_2\alpha_3\beta_4\alpha_5 \\
\varphi_f(-\tfrac{3}{2}) &= (1234;5)_{M_L=-1}\, \alpha_1\beta_2\alpha_3\beta_4\beta_5
\end{aligned} \right.
$$

T o obtain the antisymmetrized wave functions of the final state, we apply the operator: $A = A_n A_p$ to the wave functions (II-17). These antisymmetrized wave functions are given in Appendix A.

4.- Normalization factors of the initial and final state wave functions.

From (II-5) and (II-6) we have:

$$N_i^2 \langle \varphi_i \mid A^2 \varphi_i \rangle = 1$$

since A is hermitian.

A is also idempotent (4) : $A^2 = A$, therefore:

$$\text{(II-18)} \qquad N_i^2 \langle (123;45)\, \chi_i \mid A\{(123;45)\, \chi_i\} \rangle = 1$$

Similarly:

$$\text{(II-19)} \qquad N_f^2 \langle \varphi_f \mid A\varphi_f \rangle = 1$$

Now, since the normalization factors do not depend on S_z , we can choose for χ_i any one of the four spin wave functions in (II-14) and for χ_f any one of the four wave functions (II-17).

Thus:

$$N_i^2 \langle (123;45)\chi_i(\tfrac{3}{2},\tfrac{3}{2}) \mid A\{(123;45)\chi_i(\tfrac{3}{2}\,\tfrac{3}{2})\} \rangle = 1$$

Taking into account (II-14) and (II-15), and performing the spin summation, we obtain:

(II-20) $$\frac{N_i^2}{24}\left\langle (123;45) \,\middle|\, 3(123;45) - 3(124;35) - 2(523;41) + 2(524;31) - (153;42) + (154;32)\right\rangle = 1$$

But in an integral, we can exchange any two variables of integration without changing the value of the integral, provided that the integration domains of these variables are the same; thus:

(II-21) $$\left\langle (123;45) \,\middle|\, (524;31)\right\rangle = \left\langle (213;45) \,\middle|\, (514;32)\right\rangle$$

(by exchanging variables 1 and 2)

Now, since the wave function is symmetric with respect to all variables in one cluster; the order of these variables is irrelevant: hence, using the result of equation (II-21) :

$$\left\langle (123;45) \,\middle|\, (524;31)\right\rangle = \left\langle (123;45) \,\middle|\, (154;32)\right\rangle$$

Similarly:

$$\left\langle (123;45) \,\middle|\, (124;35)\right\rangle = \left\langle (123;45) \,\middle|\, (523;41)\right\rangle = \left\langle (123;45) \,\middle|\, (153;42)\right\rangle$$

Equation (II-20) therefore becomes :

(II-22) $$N_i^2 \left\langle (123;45) \,\middle|\, (123;45) - 2(124;35) + (524;31)\right\rangle = 8$$

Similarly for the final state:

(II-23) $$N_f^2 \left\langle (1234;5) \,\middle|\, (1234;5) - (5234;1)\right\rangle_{m_L=1} = 12$$

The numerical values of N_i and N_f are given in Appendix B.

In the next Chapter, while calculating the transition probability, we shall deal with integrals of the form $\langle A\varphi_f | \mathcal{O} | \varphi_i \rangle$

where $\mathcal{O}$ is some operator. The antisymmetrized wave functions $A\varphi_f$ given in Appendix A can be introduced into these integrals and the spin summation can be performed as has been done here so that the preceding matrix element is reduced to a form which contains only spatial variables.

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CHAPTER III

RADIATIVE TRANSITION PROBABILITY FROM THE (3/2+) STATE TO THE (3/2−) STATE IN He^5

1.- Introduction.

In this Chapter, we shall derive an expression for the radiative transition probability from the second excited state (3/2 +) to the ground state (3/2 −) in the He^5 nucleus.

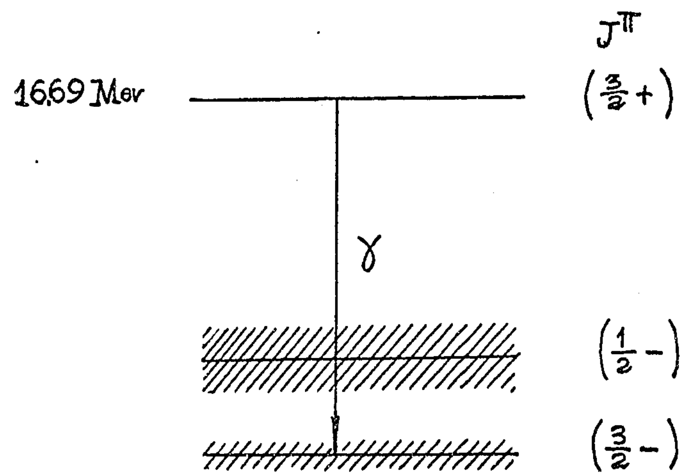

Fig.1 Energy level diagram for the He^5 nucleus

If (λ,μ) denotes the angular momentum and its z-component of the emitted photon of energy $\hbar\omega$, the transition probability from a state i to a state f is (7) :

$$T_{if}(\sigma\lambda) = \frac{8\pi\,(\lambda+1)}{\lambda[(2\lambda+1)!!]^2}\,\frac{k^{2\lambda+1}}{\hbar}\,B(\sigma\lambda) \tag{III-1}$$

where σ stands for the electric ($\sigma = E$) or magnetic ($\sigma = M$) mode of decay, and $B(\sigma\lambda)$ is the reduced matrix element:

(III-2) $$B(\sigma\lambda,\ J_i \to J_f) = \frac{1}{2J_i + 1} \sum_{M_i, M_f} |\langle f|\mathcal{O}_{\lambda\mu}|i\rangle|^2$$

$\mathcal{O}_{\lambda\mu}$ stands for the electric or magnetic multipole operator ($Q_{\lambda\mu}$ or $M_{\lambda\mu}$) :

(III-3) $$Q_{\lambda\mu} = \sum_i e_i r_i^\lambda Y_\lambda^{\mu *}(\omega_i) - i\mu_0 k(\lambda+1)^{-1} \sum_i g_{si}\, \vec{\sigma}_i \times \vec{r}_i . \nabla(r^\lambda Y_\lambda^{\mu *})_i$$

(III-4) $$M_{\lambda\mu} = \mu_0 \sum_i \left(g_{si}\, \vec{s}_i + \frac{2}{\lambda+1}\, g_{li}\, \vec{l}_i\right).\ \nabla(r^\lambda Y_\lambda^{\mu *})_i$$

In the present case, since $\pi_i \pi_f = -1$ and $J_i = J_f = 3/2$, the radiation must be of odd parity and $\lambda = |J_i - J_f|$, $|J_i - J_f| + 1$ . . . . . , $J_i + J_f = 0,1,2,3$. Therefore, the transition must be of the type E1 (we neglect the higher multipoles because their contribution is small; this point is discussed more fully in Chapter V).

With $\lambda = 1$; $J_i = J_f = 3/2$; (III-1) and (III-2) become for the electric dipole :

(III-5) $$T_{if}\ (E1) = \frac{16\pi}{9} \frac{k^3}{\hbar}\ B(E1)$$

(III-6) $$B(E1, \tfrac{3}{2} \to \tfrac{3}{2}) = \frac{1}{4} \sum_{M_i, M_f} |\langle f|\, Q_{1\mu} |i\rangle|^2$$

In equation (III-6) the selection rule requires that only one value of μ contribute to each term in the sums :

(III-7) $$\mu = M_i - M_f \qquad (\mu = 0, 1, -1)$$

2.-Calculation of T_{if}(E1).

The matrix element of the second term of the electric dipole operator $Q_{1\mu}$ (equation III-3 with $\lambda = 1$) is of the same order of magnitude as that of $M_{2\mu}$, so that it can be neglected in the calculation of T(E1). We therefore have:

(III-8) $$Q_{1\mu} \simeq eR_{1\mu}$$

where:

(III-9) $$R_{1\mu} = \sum_{3,4} r_i Y_1^{\mu *}(\omega_i)$$ (summed over all protons)

We consider now all possible terms in the sum (III-6) which contribute to B(E1). This sum is subject to two conditions:

a) The selection rule (III-7) : $\mu = M_i - M_f$

b) The spin configurations of the final and initial states must be identical. That is, if there is a "spin flip" between these states, the corresponding matrix element

M_f \ M_i	3/2	1/2	-1/2	-3/2
3/2	NO	$\mu=-1$	NO	NO
1/2	NO	$\mu=0$	$\mu=-1$	NO
-1/2	NO	$\mu=1$	$\mu=0$	NO
-3/2	NO	NO	$\mu=1$	NO

Table I

will be zero by virtue of the orthogonality of the spin wave functions of these states.

Table I indicates those terms in equation (III-6) which contribute to B(E1).

Each term of (III-6) is labelled by a pair of (M_i, M_f) values; those terms which contribute to $T_{if}(E1)$ are labelled by their μ-values in the appropriate position in the table.

The terms corresponding to $M_i = 3/2$ and $M_f = -3/2$ (second and fifth columns in the table) contribute nothing by virtue of (b). By inspecting the spin wave functions of the initial state and final state given in Chapter II, we find that there are "spin flips" between these states (see equations II-14 and II-17). For instance, the initial state with $M_i = 3/2$ has four spins "up" and one spin "down", while any possible final state has either three spins "down" and two "up", or three "up" and two "down".

The terms corresponding to $M_i = -1/2$, $M_f = 3/2$ and to $M_i = 1/2$, $M_f = -3/2$ are eliminated since their (M_i, M_f) values violate the selection rule (a).

In taking into account (III-8), equation (III-6) can now be written explicitly as follows:

$$B(E1) = \frac{e^2}{4}\Big\{ |\langle\Phi_f(\tfrac{3}{2})|R_{1-1}|\Phi_i(\tfrac{1}{2})\rangle|^2 + |\langle\Phi_f(\tfrac{1}{2})|R_{10}|\Phi_i(\tfrac{1}{2})\rangle|^2 + |\langle\Phi_f(\tfrac{1}{2})|R_{1-1}|\Phi_i(-\tfrac{1}{2})\rangle|^2 + |\langle\Phi_f(-\tfrac{1}{2})|R_{11}|\Phi_i(\tfrac{1}{2})\rangle|^2 + |\langle\Phi_f(-\tfrac{1}{2})|R_{10}|\Phi_i(-\tfrac{1}{2})\rangle|^2 + |\langle\Phi_f(-\tfrac{3}{2})|R_{11}|\Phi_i(-\tfrac{1}{2})\rangle|^2 \Big\} \tag{III-10}$$

It is emphasized here that $\Phi_i(M_i)$ and $\Phi_f(M_f)$ are respectively the antisymmetrized wave functions of the initial state and the final state.

The general term of (III-10) can also be written:

(III-11) $$\left\langle \Phi_f(M_f) \middle| R_{1\mu} \middle| \Phi_i(M_i) \right\rangle = \left\langle \varphi_f(M_f) \middle| A^{+} R_{1\mu} A \middle| \varphi_i(M_i) \right\rangle$$

φ_i and φ_f are respectively the eigenfunctions of the initial and final states, and $A = A_n A_p$ as before.

A_n and A_p commute with $R_{1\mu}$ since it is symmetric in protons and in neutrons separately; hence:

$$R_{1\mu} A = R_{1\mu} A_n A_p = A_n A_p R_{1\mu} = A R_{1\mu}$$

Equation (III-11) becomes:

(III-12) $$\left\langle \Phi_f(M_f) \middle| R_{1\mu} \middle| \Phi_i(M_i) \right\rangle = \left\langle \varphi_f(M_f) \middle| A^{+} A R_{1\mu} \middle| \varphi_i(M_i) \right\rangle$$

Since A is hermitian and idempotent:

$$A^{+} A = A^2 = A = A^{+}$$

and so (III-12) becomes:

$$\left\langle \Phi_f(M_f) \middle| R_{1\mu} \middle| \Phi_i(M_i) \right\rangle = \left\langle \varphi_f(M_f) \middle| A^{+} R_{1\mu} \middle| \varphi_i(M_i) \right\rangle$$

or:

(III-13) $$\left\langle \Phi_f(M_f) \middle| R_{1\mu} \middle| \Phi_i(M_i) \right\rangle = \left\langle \Phi_f(M_f) \middle| R_{1\mu} \middle| \varphi_i(M_i) \right\rangle$$

The calculation of the matrix element on the right hand side of equation (III-13) is clearly much simpler than that on the left hand side. This explains why separate antisymmetrizations over protons and over neutrons are preferred, as was mentionned earlier in Chapter II.

Equation (III-10) can be now written as :

(III-14) $$B(E1) = \frac{e^2}{4}\Big\{ |\langle \Phi_f(\tfrac{3}{2})|R_{1-1}|\varphi_i(\tfrac{1}{2})\rangle|^2 + |\langle \Phi_f(\tfrac{1}{2})|R_{10}|\varphi_i(\tfrac{1}{2})\rangle|^2 + |\langle \Phi_f(\tfrac{1}{2})|R_{1-1}|\varphi_i(-\tfrac{1}{2})\rangle|^2 + |\langle \Phi_f(-\tfrac{1}{2})|R_{11}|\varphi_i(\tfrac{1}{2})\rangle|^2 + |\langle \Phi_f(-\tfrac{1}{2})|R_{10}|\varphi_i(-\tfrac{1}{2})\rangle|^2 + |\langle \Phi_f(-\tfrac{3}{2})|R_{11}|\varphi_i(-\tfrac{1}{2})\rangle|^2 \Big\}$$

In order to express these matrix elements in a more explicit form in which only spatial wave functions are involved , the wave functions of the initial and final states ~~will~~ now be written out explicitly. For the initial state :

$$\varphi_i(\tfrac{1}{2}) = \frac{N_i}{\sqrt{18}}\Big[(\alpha_1\beta_3+\beta_1\alpha_3)(\alpha_2\alpha_4\beta_5+\alpha_2\beta_4\alpha_5+\beta_2\alpha_4\alpha_5) - 2\alpha_1\beta_2\alpha_3(\alpha_4\beta_5+\beta_4\alpha_5) - 2\beta_1\alpha_2\beta_3\alpha_4\alpha_5\Big](123;45)$$

$$\varphi_i(-\tfrac{1}{2}) = \frac{N_i}{\sqrt{18}}\Big[(\alpha_1\beta_3+\beta_1\alpha_3)(\alpha_2\beta_4\beta_5+\beta_2\alpha_4\beta_5+\beta_2\beta_4\alpha_5) - 2\beta_1\alpha_2\beta_3(\alpha_4\beta_5+\beta_4\alpha_5) - 2\alpha_1\beta_2\alpha_3\beta_4\beta_5\Big](123;45)$$

and for the final state:

$$\Phi_f(\tfrac{3}{2}) = \frac{N_f}{12}(\alpha_3\beta_4-\beta_3\alpha_4)\Big\{(\alpha_1\beta_2-\beta_1\alpha_2)\alpha_5(1234;5) - \alpha_1(\alpha_5\beta_2-\beta_5\alpha_2)(5234;1) + \alpha_2(\beta_1\alpha_5-\alpha_1\beta_5)(1534;2)\Big\}_{m_L=1}$$

$$\Phi_f(\tfrac{1}{2}) = \frac{N_f}{12\sqrt{3}}(\alpha_3\beta_4-\beta_3\alpha_4)\Big\{\Big[(\alpha_1\beta_2-\beta_1\alpha_2)\beta_5(1234;5) - \beta_1(\beta_2\alpha_5-\alpha_2\beta_5)(5234;1) - \beta_2(\alpha_1\beta_5-\beta_1\alpha_5)(1534;2)\Big]_{m_L=1} + \sqrt{2}\Big[(\alpha_1\beta_2-\beta_1\alpha_2)\alpha_5(1234;5) - \alpha_1(\alpha_5\beta_2-\beta_5\alpha_2)(5234;1) - \alpha_2(\alpha_1\beta_5-\beta_1\alpha_5)(1534;2)\Big]_{m_L=0}\Big\}$$

$$\Phi_f(-\tfrac{1}{2}) = \frac{N_f}{12\sqrt{3}}(\alpha_3\beta_4-\beta_3\alpha_4)\Big\{\sqrt{2}\Big[(\alpha_1\beta_2-\beta_1\alpha_2)\beta_5(1234;5) - \beta_1(\beta_2\alpha_5-\alpha_2\beta_5)(5234;1) - \beta_2(\alpha_1\beta_5-\beta_1\alpha_5)(1534;2)\Big]_{m_L=0} + \Big[(\alpha_1\beta_2-\beta_1\alpha_2)\alpha_5(1234;5) - \alpha_1(\alpha_5\beta_2-\beta_5\alpha_2)(5234;1) - \alpha_2(\alpha_1\beta_5-\beta_1\alpha_5)(1534;2)\Big]_{m_L=-1}\Big\}$$

$$\Phi_f(-\tfrac{3}{2}) = \frac{N_f}{12}(\alpha_3\beta_4-\beta_3\alpha_4)\Big\{(\alpha_1\beta_2-\beta_1\alpha_2)\beta_5\ (1234;5)$$
$$-\beta_1(\beta_2\alpha_5-\alpha_2\beta_5)(5234;1)-\beta_2(\alpha_1\beta_5-\beta_1\alpha_5)(1534;2)\Big\}_{m_L=-1}$$

From these wave functions, scalar products of the form $\langle\Phi_f|R_{1\mu}|\varphi_i\rangle$ can be formed and after carrying out the summation over spins, we obtain:

$$\langle\Phi_f(\tfrac{3}{2})|R_{1-1}|\varphi_i(\tfrac{1}{2})\rangle = \frac{N_iN_f}{6\sqrt{2}}\langle(5234;1)_1-(1234;5)_1\,|R_{1-1}|(123;45)\rangle$$

$$\langle\Phi_f(\tfrac{1}{2})|R_{10}|\varphi_i(\tfrac{1}{2})\rangle = \frac{N_iN_f}{6\sqrt{3}}\langle(5234;1)_0-(1234;5)_0\,|R_{10}|(123;45)\rangle$$

$$\langle\Phi_f(\tfrac{1}{2})|R_{1-1}|\varphi_i(-\tfrac{1}{2})\rangle = \frac{N_iN_f}{6\sqrt{6}}\langle(5234;1)_1-(1234;5)_1\,|R_{1-1}|(123;45)\rangle$$

$$\langle\Phi_f(-\tfrac{1}{2})|R_{11}|\varphi_i(\tfrac{1}{2})\rangle = \frac{N_iN_f}{6\sqrt{6}}\langle(5234;1)_{-1}-(1234;5)_{-1}\,|R_{11}|(123;45)\rangle$$

$$\langle\Phi_f(-\tfrac{1}{2})|R_{10}|\varphi_i(-\tfrac{1}{2})\rangle = \frac{N_iN_f}{6\sqrt{3}}\langle(5234;1)_0-(1234;5)_0\,|R_{10}|(123;45)\rangle$$

$$\langle\Phi_f(-\tfrac{3}{2})|R_{11}|\varphi_i(-\tfrac{1}{2})\rangle = \frac{N_iN_f}{6\sqrt{2}}\langle(5234;1)_{-1}-(1234;5)_{-1}|R_{11}|(123;45)\rangle$$

In order to simplify the preceding expressions, the following notation is introduced:

$$I_k = (-)^k\Big\langle(1234;5)_k - (5234;1)_k\Big|R_{1-k}\Big|(123;45)\Big\rangle$$

where: $$R_{1-k} = r_3Y_1^{-k*}(\omega_3) + r_4Y_1^{-k*}(\omega_4)$$

$$=(-)^k\ \big(r_3Y_1^k(\omega_3) + r_4Y_1^k(\omega_4)\big)$$

Therefore I_k becomes:

(III-15) $$I_k = \Big\langle(1234;5)_k-(5234;1)_k\Big|r_3Y_1^k(\omega_3)+r_4Y_1^k(\omega_4)\Big|(123;45)\Big\rangle$$

where: $k = 0,\ 1,\ -1$.

Taking into account equation (III-14), the reduced matrix element corresponding to the electric dipole operator has the final form :

$$B(E1) = \frac{e^2 N_i^2 N_f^2}{216} \left\{ |I_o|^2 + |I_1|^2 + |I_{-1}|^2 \right\}$$

And for the transition probability we have (equation III-5) :

$$\boxed{T(E1) = \frac{2\pi}{243} \frac{k^3}{\hbar} e^2 N_i^2 N_f^2 \left\{ |I_o|^2 + |I_1|^2 + |I_{-1}|^2 \right\}} \qquad \text{(III-16)}$$

*

* *

In this Chapter, we have derived an expression for the transition probability for gamma emission in He^5 (equation III-16). This expression is particularly simple, for it is a function of only one kind of integral I_k (see equation III-15).

The next Chapter will be devoted to the evaluation of I_k and thence the value of T(E1).

CHAPTER IV

METHOD OF CALCULATION OF THE INTEGRAL I_k .

In the last Chapter, the final formula for the transition probability T(E1) was found to involve only one type of integral, which was designated by I_k:

(IV-1) $$I_k = \left\langle (1234;5)_{m_2=k} - (5234;1)_{m_1=k} \middle| r_3 Y_1^k(\omega_3) + r_4 Y_1^k(\omega_4) \middle| (123;45) \right\rangle$$

In fact, in the matrix element (IV-1) , the operator $(r_3 Y_1^k(\omega_3) + r_4 Y_1^k(\omega_4))$ must be expressed in relative coordinates: that is $\bar{r}_3 Y_1^k(\bar{\omega}_3) + \bar{r}_4 Y_1^k(\bar{\omega}_4)$ (where: $\vec{\bar{r}}_i = \vec{r}_i - \vec{R}_{cm}$) since in the expression for the electric multipole $Q_{\lambda\mu}$ (equation III-3), the spatial coordinates are referred to the center-of-mass of the nucleus.

Therefore, (IV-1) becomes:

(IV-2) $$I_k = \left\langle (1234;5)_k - (5234;1)_k \middle| \bar{r}_3 Y_1^k(\bar{\omega}_3) + \bar{r}_4 Y_1^k(\bar{\omega}_4) \middle| (123;45) \right\rangle$$

or:

(IV-3) $$I_k = A_k - B_k$$

where:

(IV-4) $$A_k = \left\langle (1234;5)_k \middle| \bar{r}_3 Y_1^k(\bar{\omega}_3) + \bar{r}_4 Y_1^k(\bar{\omega}_4) \middle| (123;45) \right\rangle$$

(IV-5) $$B_k = \left\langle (5234;1)_k \middle| \bar{r}_3 Y_1^k(\bar{\omega}_3) + \bar{r}_4 Y_1^k(\bar{\omega}_4) \middle| (123;45) \right\rangle .$$

We shall demonstrate the evaluation of A_k in full detail here; that of B_k is similar and only the result will therefore be written.

1.- Evaluation of A_k.

The wave function for the initial state is :

$$\text{(IV-6)}\quad (123;45) = \exp\left\{-\frac{\alpha}{2}\sum_{i=1}^{3} r_i'^2 - \frac{\bar{\alpha}}{2}\sum_{j=4}^{5} r_j'^2\right\} R^2 e^{-\frac{3\beta}{5}R^2}\, e^{-\frac{5\gamma}{2}R_{cm}^2}$$

where $\vec{r_i'}$ and $\vec{r_j'}$ are respectively relative coordinates of the ith and jth particles in the triton and deuteron clusters:

$$\vec{r_i'} = \vec{r_i} - \vec{R_t} \quad (i=1,2,3) \quad ; \quad \vec{r_j'} = \vec{r_j} - \vec{R_d} \quad (j=4,5)$$

$$\vec{R_t} = 1/3\ (\vec{r_1} + \vec{r_2} + \vec{r_3}) \quad ; \quad \vec{R_d} = \tfrac{1}{2}(\vec{r_4} + \vec{r_5})$$

$\vec{R} = \vec{R_t} - \vec{R_d}$ is the relative coordinate of the two clusters, and $\vec{R_{cm}}$ is the coordinate of the center-of-mass of the whole system.

The wave function for the final state is:

$$\text{(IV-7)}\quad (1234;5)_{m_l=k} = \exp\left\{-\frac{\alpha_1}{2}\sum_{i=1}^{4} r_i''^2\right\} R_1 Y_1^k(\Omega_1)\, e^{-\frac{2\beta'}{5}R_1^2}\, e^{-\frac{5\gamma}{2}R_{cm}^2}$$

where: $\vec{r_i''} = \vec{r_i} - \vec{R_\alpha} \quad (i=1,2,3,4)$

$$\vec{R_\alpha} = \tfrac{1}{4}(\vec{r_1} + \vec{r_2} + \vec{r_3} + \vec{r_4})$$

$$\vec{R_1} = \vec{R_\alpha} - \vec{r_5}$$

.We have included in (IV-6) and (IV-7) the wave function of the center-of-mass of the nucleus $e^{-\frac{5\gamma}{2}R_{cm}^2}$ -which, in fact must be discarded, because the center-of-mass moves like a free particle rather than in a harmonic potential. It has been included here only because A_k and B_k must be integrated over five variables $\vec{r_1}, \vec{r_2}, \vec{r_3}, \vec{r_4}, \vec{r_5}$ (and not four), so the center-of-mass coordinate $\overrightarrow{R_{cm}}$ must be added to the four internal and relative coordinates to give the system five degrees of freedom. It will be shown later that this center-of-mass wave function can always be separated from the integrals A_k and B_k so that it does not enter essentially into the calculation of A_k and B_k.

Expressing now (IV-6) and (IV-7) in terms of variables $\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{r}_5$ and bringing these wave functions into (IV-4), we obtain:

$$\text{(IV-8)} \qquad A_k = \int e^{-\phi} R_1 Y_1^{k*}(\Omega_1) R^2 \left(\bar{r}_3 Y_1^k(\bar{\omega}_3) + \bar{r}_4 Y_1^k(\bar{\omega}_4) \right) e^{-5\gamma R_{cm}^2} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

where:

$$\text{(IV-9)} \qquad \phi = A(r_1^2 + r_2^2 + r_3^2) + Br_4^2 + Cr_5^2 + 2D(\vec{r}_1\vec{r}_2 + \vec{r}_2\vec{r}_3 + \vec{r}_3\vec{r}_1)$$
$$+ 2(E\vec{r}_4 + F\vec{r}_5)(\vec{r}_1 + \vec{r}_2 + \vec{r}_3) + 2G\vec{r}_4\vec{r}_5$$

The values of A,B,C,. . . . G are listed in table III, Appendix C.

In order to integrate A_k , we find a linear transformation from the set of variables $(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{r}_5)$ to the new variables $(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3, \vec{\rho}_4, \vec{R}_{cm})$ such that ϕ can be expressed as a sum of square terms of these new variables. This work has been performed in Appendix C, and the result is (formula C-16) :

$$\text{(IV-10)} \qquad \phi = L\rho_1^2 + M\rho_2^2 + \rho_3^2 + \rho_4^2$$

where:

$$\vec{\rho}_1 = \vec{R}_1 = \tfrac{1}{4}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_5$$
$$\vec{\rho}_2 = \vec{r}_1 - \vec{r}_2$$
$$\text{(IV-11)} \qquad \vec{\rho}_3 = X(\vec{r}_1 + \vec{r}_2 + \vec{r}_3) + Y\vec{r}_4 + Z\vec{r}_5$$
$$\vec{\rho}_4 = S(\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3)$$

Note that ϕ contains only four square terms (equation IV-10); since it does not include the center-of-mass coordinate; it has therefore only four independent variables associated with it.

In term of the new variables, A_k becomes :

(IV-12) $$A_k = |J|^3 \int exp(-L\rho_1^2 - M\rho_2^2 - \rho_3^2 - \rho_4^2) \times \rho_1 Y_1^{k*}(\Omega_1)\left(\overline{r}_3 Y_1^k(\overline{\omega}_3) + \overline{r}_4 Y_1^k(\overline{\omega}_4)\right) e^{-5\gamma R_{cm}^2} \, d\vec{\rho}_1 \, d\vec{\rho}_2 \, d\vec{\rho}_3 \, d\vec{\rho}_4 \, d\vec{R}_{cm}$$

where J is the jacobian of the transformation:

(IV-13) $$J = \frac{\partial(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{r}_5)}{\partial(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3, \vec{\rho}_4, \vec{R}_{cm})} = \frac{2}{3S(X-Y)}$$

On the other hand, we have :

(IV-14) $$\vec{r}_3 + \vec{r}_4 = a\vec{\rho}_1 + b\vec{\rho}_3 + c\vec{\rho}_4$$

where:

(IV-15) $$a = \frac{4}{15}\,\frac{6X-Z}{X-Y} \quad ; \quad b = -\frac{2}{3(X-Y)} \quad ; \quad c = -\frac{1}{3S}$$

From (IV-14) we deduce that :

(IV-16) $$\overline{r}_3 Y_1^k(\overline{\omega}_3) + \overline{r}_4 Y_1^k(\overline{\omega}_4) = a\rho_1 Y_1^k(\Omega_1) + b\rho_3 Y_1^k(\Omega_3) + c\rho_4 Y_1^k(\Omega_4)$$

Also, we have :

$$\vec{R} = d\vec{\rho}_1 + e\vec{\rho}_3$$

(IV-17) $$d = \frac{2}{3}\,\frac{Y-Z}{Y-X} \quad ; \quad e = \frac{5}{6(X-Y)}$$

Hence:

(IV-18) $$R^2 = d^2\rho_1^2 + e^2\rho_3^2 + 2de\rho_1\rho_3\cos\theta_{13}$$

θ_{13} is angle between the directions $\vec{\rho}_1$ and $\vec{\rho}_3$, and we have :

(IV-19) $$\cos\theta_{13} = \frac{4\pi}{3}\sum_{m=-1}^{1} Y_1^m(\Omega_1)\, Y_1^{m*}(\Omega_3)$$

Bringing now (IV-16) and (IV-18) into (IV-12), we obtain :

(IV-20) $$A_k = |J|^3 \int e^{-5\gamma R_{cm}^2}\, d\vec{R}_{cm} \int e^{-(I\rho_1^2 + M\rho_2^2 + \rho_3^2 + \rho_4^2)}\, \rho_1 y_1^{k*}(\Omega_1) \times \left(a\rho_1 y_1^k(\Omega_1) + b\rho_3 y_1^k(\Omega_3) + c\rho_4 y_1^k(\Omega_4)\right)\left(d^2\rho_1^2 + e^2\rho_3^2 + 2de\rho_1\rho_3 \cos\theta_{13}\right) d\vec{\rho}_1\, d\vec{\rho}_2\, d\vec{\rho}_3\, d\vec{\rho}_4$$

In equation (IV-20), we can now drop the "center-of-mass integral" $\int e^{-5\gamma R_{cm}^2}\, d\vec{R}_{cm}$, for this integral is also figured in the normalization constants (see Appendix B).

A_k can now be written as a sum of simpler integrals:

(IV-21) $$A_k = |J|^3 (A_1 + A_2 + A_3 + A_4)$$

where A_n is integral of the form :

$$A_n = \int e^{-\phi} \rho_1 y_1^{k*}(\Omega_1) f_n(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3, \vec{\rho}_4)\, d\vec{\rho}_1\, d\vec{\rho}_2\, d\vec{\rho}_3\, d\vec{\rho}_4$$

and:

$$f_1 = a\rho_1 Y_1^k(\Omega_1)(d^2\rho_1^2 + e^2\rho_3^2)$$

$$f_2 = (b\rho_3 Y_1^k(\Omega_3) + c\rho_4 Y_1^k(\Omega_4))(d^2\rho_1^2 + e^2\rho_3^2)$$

$$f_3 = 2de\rho_1\rho_3\cos\theta_{13}(a\rho_1 Y_1^k(\Omega_1) + c\rho_4 Y_1^k(\Omega_4))$$

$$f_4 = 2de\rho_1\rho_3\cos\theta_{13}\, b\rho_3 Y_1^k(\Omega_3)$$

We can see easily that $A_2 = A_3 = 0$, since they contain integrals of the form: $\int y_1^k(\Omega_i)\, d\Omega_i = 0$

The integrations of A_1 and A_4 are now straightforward:

$$A_1 = ad^2\int e^{-L\rho_1^2}\rho_1^6\, d\rho_1 \int e^{-M\rho_2^2} d\vec{\rho_2} \int e^{-\rho_3^2} d\vec{\rho_3} \int e^{-\rho_4^2} d\vec{\rho_4}$$
$$+ ae^2\int e^{-L\rho_1^2}\rho_1^4\, d\rho_1 \int e^{-M\rho_2^2} d\vec{\rho_2} \int e^{-\rho_3^2}\rho_3^2\, d\vec{\rho_3} \int e^{-\rho_4^2} d\vec{\rho_4}$$

$$A_1 = \frac{3a\pi^5}{16\, L^{7/2} M^{3/2}}\,(5d^2 + 3e^2 L)$$

$$A_4 = \frac{8\pi bde}{3}\int e^{-L\rho_1^2}\rho_1^4\, d\rho_1 \int e^{-M\rho_2^2} d\vec{\rho_2} \int e^{-\rho_3^2}\rho_3^4\, d\rho_3 \int e^{-\rho_4^2} d\vec{\rho_4}$$
$$= \frac{3bde\pi^5}{8L^{5/2}M^{3/2}}$$

Finally, (IV-21) gives :

$$A_k = |J|^3 (A_1 + A_4)$$

(IV-22) $$\boxed{A_k = \frac{\pi^5(5ad^2 + 3ae^2L + 2bdeL)}{18|S(X-Y)|^3\, L^{7/2} M^{3/2}}}$$

2.- <u>Evaluation of B_k</u>.-

(IV-23) $$B_k = \int e^{-\phi'} R_1' y_1^{k*}(\Omega_1') R^2\left(\vec{r}_3 y_1^k(\omega_3) + \vec{r}_4 y_1^k(\omega_4)\right) e^{-5\gamma R_{cm}^2} \times d\vec{r_1}\, d\vec{r_2}\, d\vec{r_3}\, d\vec{r_4}\, d\vec{r_5}$$

where:

$$\vec{R_1'} = \tfrac{1}{4}(\vec{r_2} + \vec{r_3} + \vec{r_4} + \vec{r_5}) - \vec{r_1}$$

$$\phi' = A' r_1^2 + B'(r_2^2 + r_3^2) + C'(r_4^2 + r_5^2) + 2\vec{r_1}\cdot\left[D'(\vec{r_2} + \vec{r_3}) + E'(\vec{r_4} + \vec{r_5})\right]$$
$$+ 2F'\vec{r_2}\vec{r_3} + 2G'\vec{r_4}\vec{r_5} + 2H'(\vec{r_2} + \vec{r_3})\cdot(\vec{r_4} + \vec{r_5})$$

The values of $A', B', \ldots . H'$ are listed in Table I, Appendix C. In this appendix, it is also shown that:

$$\phi' = L'\rho_1^2 + M'\rho_2^2 + N'\rho_3^2 + P'\rho_4^2$$

where:

$$\vec{\rho_1} = \vec{R_1'} = \tfrac{1}{4}(\vec{r_2}+\vec{r_3}+\vec{r_4}+\vec{r_5}) - \vec{r_1}$$

$$\vec{\rho_2} = \vec{r_4} - \vec{r_5}$$

$$\vec{\rho_3} = \vec{r_2} - \vec{r_3}$$

$$\vec{\rho_4} = X'\vec{r_1} + Y'(\vec{r_2}+\vec{r_3}) + Z'(\vec{r_4}+\vec{r_5})$$

In terms of the new variables, (IV-23) becomes:

(IV-24) $$B_k = \frac{1}{|Z'-Y'|^3} \int \exp\left(-L'\rho_1^2 - M'\rho_2^2 - N'\rho_3^2 - P'\rho_4^2\right) \rho_1 Y_1^{k*}(-\Omega_1) \left(c'^2\rho_1^2 + d'^2\rho_4^2 + 2c'd'\rho_1\rho_4 \cos\theta_{14}\right)\left(\tfrac{2}{5}\rho_1 Y_1^k(-\Omega_1) + \tfrac{1}{2}\rho_2 Y_1^k(\Omega_2) - \tfrac{1}{2}\rho_3 Y_1^k(\Omega_3)\right) d\vec{\rho_1}\, d\vec{\rho_2}\, d\vec{\rho_3}\, d\vec{\rho_4}$$

(we have dropped the integral $\int e^{-5\gamma R_{cm}^2} d\vec{R_{cm}}$ in this expression for the same reason as it was dropped in the expression for A_k).

where:

$$c' = \frac{2}{3}\,\frac{X'-Y'}{Y'-Z'} \qquad d' = \frac{5}{6(Y'-Z')}$$

The integration of (IV-24) is similar to that of A_k and we get the following result:

(IV-25) $$\boxed{B_k = \frac{3\pi^5\left(c'^2P' + 3/5\, d'^2L'\right)}{8\,|Z'-Y'|^3 (M'N')^{3/2}\, L'^{7/2}\, P'^{5/2}}}$$

*

* *

From equations (IV-22) and (IV-25), the value of the matrix element I_k can be calculated by taking into account equation (IV-3). It is noted here that I_k does not depend on the value of k, so that :

$$I_o = I_1 = I_{-1}$$

This will simplify greatly the expression for T(E1) given in Chapter III.

CHAPTER V

NUMERICAL ANALYSIS AND CONCLUSIONS

The following expression was derived in Chapter III for the probability of the transition in He^5 with which we are concerned here:

$$T(E1) = \frac{2\pi}{243}\frac{k^3}{\hbar} e^2 N_i^2 N_f^2 \left(|I_0|^2 + |I_1|^2 + |I_{-1}|^2 \right) \tag{V-1}$$

In Chapter IV, the integral I_k $(k = 0,1,-1)$ was evaluated, and it was found that I_k is independent of k; equation (V-1) becomes therefore:

$$T(E1) = \frac{2\pi}{81}\frac{k^3}{\hbar} e^2 N_i^2 N_f^2 |I_k|^2 \tag{V-2}$$

We now calculate T(E1) numerically.

1.- Numerical calculation of T(E1).

We shall use here the numerical values of the width parameters given by Pearlstein, Tang and Wildermuth (6). These parameters were determined by these authors by a variational method in a calculation of the first three energy levels of the He^5 nucleus.

We shall denote by α, $\bar{\alpha}$, α_1 the width parameters of the harmonic oscillator potentials for the motion internal to the triton, deuteron and alpha-particle clusters, and by β and β' those associated with the relative motion of the "triton-deuteron" clusters and the "alpha-neutron" clusters respectively.

The numerical values of these parameters are given in Table I.

α	2.81×10^{25} cm^{-2}
$\bar{\alpha}$	4.78×10^{25} cm^{-2}
β	0.422×10^{25} cm^{-2}
α_1	4.33×10^{25} cm^{-2}
β'	$\left.\begin{matrix}2.25\\3.25\end{matrix}\right\} \times 10^{25}$ cm^{-2}

Table I

Note that there are two possible values of β'; these arise from two possible choices for the range and the depth of the spin-orbit potential used in (6); both gives equally good agreement with the positions of the energy levels. There will therefore be two numerical values for I_k, and as many for T(E1).

<u>Evaluation of I_k.</u>

(V-3) $$I_k = A_k - B_k$$

where:

(V-4) $$A_k = \frac{\pi^5 \; (5ad^2 + 3ae^2L + 2bdeL)}{18\,|S(X-Y)|^3 \; L^{7/2} \; M^{3/2}}$$

(V-5) $$B_k = \frac{3\pi^5 \; (c'^2P' + 3/5 \; d'^2L')}{8\,|Z'-Y'|^3 \, (M'N')^{3/2} \; L'^{7/2} \; P'^{5/2}}$$

a	0.229
b	$0.323 \times 10^{-12.5}$ cm
d	0.713
e	$-0.404 \times 10^{-12.5}$ cm
L	1.88×10^{25} cm^{-2} 2.28×10^{25} cm^{-2}
M	1.79×10^{25} cm^{-2}
X	$-0.384 \times 10^{12.5}$ cm^{-1}
Y	$1.68 \times 10^{12.5}$ cm^{-1}
S	$0.772 \times 10^{12.5}$ cm^{-1}

Table II

c'	-0.462
d'	0.162×10^{-25} cm^{2}
L'	1.80×10^{25} cm^{-2} 2.20×10^{25} cm^{-2}
M'	2.28×10^{25} cm^{-2}
N'	1.79×10^{25} cm^{-2}
P'	0.097×10^{-25} cm^{2}
Y'	2.77×10^{25} cm^{-2}
Z'	-2.38×10^{25} cm^{-2}

Table III

The numerical values of the parameters a, b, . . . X, Y . . . etc in the expressions for A_k and B_k are listed in Tables II and III. Whenever these parameters depend on β', two entries appear in the tables.

Inserting these numerical values into (V-4) and (V-5), we obtain :

$$A_k = \begin{cases} 8.58 \times 10^{-202} \; cm^{16} \\ 4.09 \times 10^{-202} \; cm^{16} \end{cases}$$

and:

$$B_k = \begin{cases} 21.64 \times 10^{-202} \; cm^{16} \\ 12.13 \times 10^{-202} \; cm^{16} \end{cases}$$

Hence:

$$(V\text{-}6) \qquad I_k = \begin{cases} -1.306 \times 10^{-201} \ \mathrm{cm}^{16} \\ -0.804 \times 10^{-201} \ \mathrm{cm}^{16} \end{cases}$$

We have now all the numerical values necessary for the calculation of T(E1) :

$$k = \frac{E}{\hbar c} = 8.45 \times 10^{11} \ \mathrm{cm}^{-1} \qquad (E = 16.69 \ \mathrm{Mev.})$$

N_i^2 , N_f^2 are calculated in Appendix B :

$$N_i^2 = 3.03 \times 10^{197} \ \mathrm{cm}^{-16}$$

$$N_f^2 = \begin{cases} 3.50 \times 10^{176} \ \mathrm{cm}^{-14} \\ 8.45 \times 10^{176} \ \mathrm{cm}^{-14} \end{cases}$$

Finally, taking into account equation (V-2) , we obtain the following results :

$$(V\text{-}7) \qquad T(E1) = \begin{cases} 1.85 \times 10^{15} \ \mathrm{sec}^{-1} \\ 1.70 \times 10^{15} \ \mathrm{sec}^{-1} \end{cases}$$

The level width Γ_γ for electric dipole γ-emission is related to the transition probability by the equation:

$$\Gamma_\gamma = 0.66 \times 10^{-15} \ T(E1) \quad \mathrm{ev.}$$

Hence:

$$(V\text{-}8) \qquad \Gamma_\gamma = \begin{cases} 1.23 \ \mathrm{ev} \\ 1.12 \ \mathrm{ev} \end{cases}$$

2.- Conclusion.

The calculated level widths (V-8) can now be compared with the experimental results. In the actual experimental situation, no accurate measurement of this width exists yet, presumably because of the relative sharpness of the energy level at 16.69 Mev. However, some rough estimates of the level width can be deduced from the $T(d,\gamma)He^5$ and $T(d,n)He^4$ experiments:

G.A. Sawyer and L.C. Burkhardt (12) have determined a lower limit for the yield ratio of neutrons to gamma rays as 10^4. The neutron level width Γ_n of the 16.69 Mev state in the He^5 compound nucleus for the $T(d,n)He^4$ reaction is quoted in this work to be 66 kev, so that:

$$\Gamma_\gamma < 6.6 \text{ ev}$$

A more recent study by J.H. Coon and R.W. Davis (13) indicates that the yield ratio of gamma rays to neutrons from the $T(d,n)He^4$ reaction is about 2×10^{-5}. Using the same values of Γ_n as above, we deduced that:

$$\Gamma_\gamma \simeq 1.32 \text{ ev}$$

Thus, the calculated level width agrees quite closely with the experimental result.

A calculation of the transition probability based on the single particle model is carried out in order to show how the description of the He^5 nucleus is improved by the cluster model.

The γ -decay transition probability for a single proton (see fig.1) can be written in a general form as (8);

$$T_{sp}(E1) = \frac{4.4(L+1)}{L[(2L+1)!!]^2}\left(\frac{3}{L+3}\right)^2\left(\frac{\hbar\omega}{197\,\mathrm{Mev}}\right)^2 \times (a \text{ in } 10^{-13}\mathrm{cm})^{2L} S(J_i,L,J_f) \times 10^{21}\,\mathrm{sec}^{-1}$$

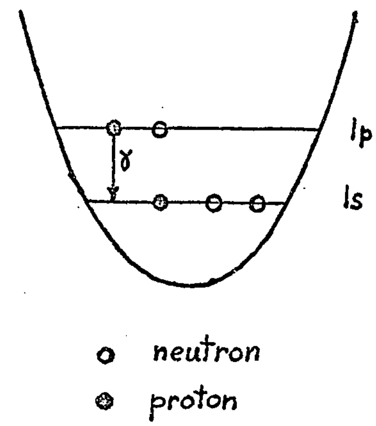

Fig.1 The radiative transition in the He^5 nucleus from the (3/2+) state to the (3/2 -) state is due to the jump of one proton from the 1p state to the 1s state.

where a is the radius of the nucleus and is assumed to be $1.2\ A^{\frac{1}{3}} \times 10^{-13}$ cm, and $S(J_i,L,J_f)$ is the statistical factor:

$$S(J_i,L,J_f) = (2J_f+1)\left[\langle J_i J_f \tfrac{1}{2} -\tfrac{1}{2} | L0 \rangle\right]^2$$

Numerically:

$$T_{sp}(E1) = 2.8 \times 10^{17}\ \mathrm{sec}^{-1}$$

This value is about one hundred times bigger than the transition probability obtained using the cluster model. The reduction of the "cluster model transition probability" $T_{cm}(E1)$ is due partly to the cluster model wave functions and partly to the fact that the single-particle wave functions are not antisymmetrized : a calculation using the unantisymmetrized cluster model wave functions gives $T(E1) = 12.7 \times 10^{15}\ \mathrm{sec}^{-1}$ and $8.3 \times 10^{15}\ \mathrm{sec}^{-1}$, which are factors of 8 and 5 larger than the value obtained using antisymmetrized cluster model wave functions.

We mention for the sake of completeness that we have also calculated the contributions of the spin term of the electric dipole operator and the magnetic quadrupole operator to the transition probability in the case where there is no contribution of the principal (orbital) term of $Q_{1\mu}$ (see page 10, Chapter II). In this calculation, the set (II-10) of spin wave functions for the triton is used. The result is that $T(E1) + T(M2)$ is about $4 \times 10^{13}\ \mathrm{sec}^{-1}$, which is fifty times smaller than the value given by equation (V-7). This verifies the fact mentioned in Chapter II that the first term of $Q_{1\mu}$ is predominantly responsible for the transition in He^5.

Finally, an alternative method of calculation of the transition probability can be suggested: H.A. Bethe and E.E. Salpeter (14) have shown that if exact nuclear wave functions are used, the operator $\vec{r}$ in the electric dipole operator can be replaced by $\frac{i}{mck}\vec{p}$, where $\vec{p}$ is the momentum operator and m is the mass of the proton. Thus:

(V-9) $$Q_{1\mu} \simeq e \sum_{3,4} r_i Y_1^{\mu *}(\omega_i)$$

becomes :

(V-10) $$Q'_{1\mu} \simeq \frac{ie}{mck} \sum_{3,4} p_i Y_1^{\mu *}(\omega_{pi})$$

This method provides us with a test for the cluster model wave functions, because if our chosen wave functions are exact, the matrix elements of $Q_{1\mu}$ and $Q'_{1\mu}$ must be the same, and so are the transition probabilities. However, since we are using model wave functions here, it is clear that the difference between the two results will provide a measure of the deviation of the cluster model wave functions from the exact nuclear wave functions. Such a calculation would be well worth performing, since the present result seems to vindicate that the cluster model provides quite an accurate description of the He^5 nucleus.

APPENDIX A

ANTISYMMETRIZED WAVE FUNCTIONS OF THE FINAL STATE

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In the following expressions, Φ denotes the antisymmetrized wave function and the number between the parentheses of Φ denotes the z-component of the total spin of the nucleus.

$$\Phi_f\left(\tfrac{3}{2}\right) = \frac{N_f}{3!\,2!}\,(\alpha_3\beta_4 - \beta_3\alpha_4)\Big\{(\alpha_1\beta_2 - \beta_1\alpha_2)\alpha_5\,(1234;5) - \alpha_1(\beta_2\alpha_5 - \alpha_2\beta_5)(5234;1) + \alpha_2(\beta_1\alpha_5 - \alpha_1\beta_5)(1534;2)\Big\}_{m_L=1}$$

$$\Phi_f\left(\tfrac{1}{2}\right) = \frac{N_f}{3!\,2!\sqrt{3}}\,(\alpha_3\beta_4 - \beta_3\alpha_4)\Big\{\big[(\alpha_1\beta_2 - \beta_1\alpha_2)\beta_5\,(1234;5) - \beta_1(\beta_2\alpha_5 - \alpha_2\beta_5)(5234;1) + \beta_2(\beta_1\alpha_5 - \alpha_1\beta_5)(1534;2)\big]_{m_L=1}$$
$$+\sqrt{2}\big[(\alpha_1\beta_2 - \beta_1\alpha_2)\alpha_5\,(1234;5) - \alpha_1(\beta_2\alpha_5 - \alpha_2\beta_5)(5234;1) - \alpha_2(\alpha_1\beta_5 - \beta_1\alpha_5)(1534;2)\big]_{m_L=0}\Big\}$$

$$\Phi_f\left(-\tfrac{1}{2}\right) = \frac{N_f}{3!\,2!\sqrt{3}}\,(\alpha_3\beta_4 - \beta_3\alpha_4)\Big\{\sqrt{2}\big[(\alpha_1\beta_2 - \beta_1\alpha_2)\beta_5\,(1234;5) - \beta_1(\beta_2\alpha_5 - \alpha_2\beta_5)(5234;1) - \beta_2(\alpha_1\beta_5 - \beta_1\alpha_5)(1534;2)\big]_{m_L=0}$$
$$+\big[(\alpha_1\beta_2 - \beta_1\alpha_2)\alpha_5\,(1234;5) - \alpha_2(\alpha_1\beta_5 - \beta_1\alpha_5)(1534;2) - \alpha_1(\beta_2\alpha_5 - \alpha_2\beta_5)(5234;1)\big]_{m_L=-1}\Big\}$$

$$\Phi_f\left(-\tfrac{3}{2}\right) = \frac{N_f}{3!\,2!}\,(\alpha_3\beta_4 - \beta_3\alpha_4)\Big\{(\alpha_1\beta_2 - \beta_1\alpha_2)\beta_5\,(1234;5) - \beta_1(\beta_2\alpha_5 - \alpha_2\beta_5)(5234;1) - \beta_2(\alpha_1\beta_5 - \beta_1\alpha_5)(1534;2)\Big\}_{m_L=}$$

APPENDIX B

CALCULATION OF THE NORMALIZATION CONSTANTS

Let rewrite equations (II-22),(II-23) which determine the normalization constants N_i , N_f of the initial and final state wave functions:

(B-1) $$N_i^2 \langle (123;45) | (123;45) - 2(124;35) + (524;31) \rangle = 8$$

(B-2) $$N_f^2 \langle (1234;5) | (1234;5) - (5234;1) \rangle_{m_L=1} = 12$$

1.- Evaluation of N_i.

We now calculate the three integrals:

$$I_1 = \langle (123;45) | (123;45) \rangle$$

$$I_2 = \langle (123;45) | (124;35) \rangle$$

$$I_3 = \langle (123;45) | (524;31) \rangle$$

(a) $$I_1 = \int e^{-\phi} R^4 \exp\left(-\frac{6\beta R^2}{5}\right) e^{-5\gamma R_{cm}^2} \, d\vec{r}_1 \, d\vec{r}_2 \, d\vec{r}_3 \, d\vec{r}_4 \, d\vec{r}_5$$

where ϕ can be written as:

$$\phi = \frac{2\alpha}{3} \rho_1^2 + \frac{\alpha}{2} \rho_2^2 + \frac{\bar{\alpha}}{2} \rho_3^2$$

and:
$$\vec{\rho}_1 = \vec{r}_1 - \tfrac{1}{2}(\vec{r}_2 + \vec{r}_3)$$
$$\vec{\rho}_2 = \vec{r}_2 - \vec{r}_3$$
$$\vec{\rho}_3 = \vec{r}_4 - \vec{r}_5$$
$$\vec{R} = 1/3(\vec{r}_1 + \vec{r}_2 + \vec{r}_3) - \tfrac{1}{2}(\vec{r}_4 + \vec{r}_5)$$

In terms of the new coordinates $(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3, \vec{R}, \vec{R}_{cm})$ I_1 becomes:

(B-3) $$I_1 = |J|^3 \int exp\left\{-\frac{2\alpha}{3}\rho_1^2 - \frac{\alpha}{2}\rho_2^2 - \frac{\bar{\alpha}}{2}\rho_3^2 - \frac{6\beta}{5}R^2\right\} R^4 \times d\vec{\rho_1}\, d\vec{\rho_2}\, d\vec{\rho_3}\, d\vec{R} \times \int e^{-5\gamma R_{cm}^2}\, d\vec{R}_{cm}$$

where:

$$J = \frac{\partial(\vec{r_1},\vec{r_2},\vec{r_3},\vec{r_4},\vec{r_5})}{\partial(\vec{\rho_1},\vec{\rho_2},\vec{\rho_3},\vec{R},\vec{R}_{cm})} = -1$$

The evaluation of I_1 is now straightforward since I_1 can be separated in four "single variable" integrals. Hereafter, the "center-of-mass integral" $\int e^{-5\gamma R_{cm}^2} d\vec{R}_{cm}$ can be dropped for the reason we have pointed out in Chapter IV.

(B-4) $$I_1 = \frac{5^{9/2}}{48}\frac{\pi^6}{\alpha^3 \bar{\alpha}^{3/2} \beta^{7/2}}$$

(b)

(B-5) $$I_2 = \int e^{-\phi_1} R^2 R_1^2\, e^{-5\gamma R_{cm}^2}\, d\vec{r_1}\, d\vec{r_2}\, d\vec{r_3}\, d\vec{r_4}\, d\vec{r_5}$$

where:

$$R_1 = 1/3\ (\vec{r_1}+\vec{r_2}+\vec{r_4}) - \tfrac{1}{2}(\vec{r_3}+\vec{r_5})$$

and;

$$\phi_1 = A_1(r_1^2+r_2^2) + B_1(r_3^2+r_4^2) + C_1 r_5^2 + 2D_1\vec{r_1}\vec{r_2} + 2E_1(\vec{r_1}+\vec{r_2})(\vec{r_3}+\vec{r_4}) + 2F_1\vec{r_3}\vec{r_4} + 2\left[F_1(\vec{r_1}+\vec{r_2}) + G_1(\vec{r_3}+\vec{r_4})\right]\cdot\vec{r_5}$$

Coefficients A_1, B_1 . . . . G_1 are given in Table I along with their numerical values.

Substituting the following change of variables in (B-5):

$$\vec{\rho_1} = \vec{r_1} - \vec{r_2}$$
$$\vec{\rho_2} = \vec{r_3} - \vec{r_4}$$

$$\vec{\rho_3} = \vec{r_1} + \vec{r_2} - \vec{r_3} - \vec{r_4}$$

$$\vec{\rho_4} = C_1\vec{r_5} + F_1(\vec{r_1}+\vec{r_2}) + G_1(\vec{r_3}+\vec{r_4})$$

$$\vec{R}_{cm} = 1/5\ (\vec{r_1}+\vec{r_2}+\vec{r_3}+\vec{r_4}+\vec{r_5})$$

A_1	$\frac{2\alpha}{3} + \frac{2\beta}{15}$	1.93×10^{25} cm^{-2}
B_1	$\frac{\alpha}{3} + \frac{\overline{\alpha}}{4} + \frac{13\beta}{60}$	2.22×10^{25} cm^{-2}
C_1	$\frac{\overline{\alpha}}{2} + \frac{3\beta}{10}$	2.52×10^{25} cm^{-2}
D_1	$-\frac{\alpha}{3} + \frac{2\beta}{15}$	-0.881×10^{25} cm^{-2}
E_1	$-\left(\frac{\alpha}{6} + \frac{\beta}{30}\right) = -\frac{A_1}{4}$	-0.483×10^{25} cm^{-2}
F_1	$-\frac{\beta}{5}$	-0.0843×10^{25} cm^{-2}
G_1	$-\frac{\overline{\alpha}}{4} + \frac{\beta}{20}$	-1.17×10^{25} cm^{-2}

Table I

we obtain:

(B-6)
$$I_2 = \frac{1}{8C_1^3}\int \exp\left(-L\rho_1^2 - M\rho_2^2 - N\rho_3^2 - P\rho_4^2\right)\left(a\vec{\rho_2} + b\vec{\rho_3} + c\vec{\rho_4}\right)^2 \times\left(-a\vec{\rho_2} + b\vec{\rho_3} + c\vec{\rho_4}\right)^2 d\vec{\rho_1}\, d\vec{\rho_2}\, d\vec{\rho_3}\, d\vec{\rho_4}$$

where: $L = \frac{1}{2}(A_1 - D_1)$; $M = \frac{1}{2}(B_1 - F_1)$; $N = \frac{F_1 G_1}{C_1} - E_1$; $P = \frac{1}{C_1}$

$a = 5/12$; $b = -\frac{F_1 + 4G_1}{6C_1}$; $c = -\frac{1}{2C_1}$

Integration of (B-6) over $\vec{\rho_1}, \vec{\rho_2}, \vec{\rho_3}, \vec{\rho_4}$ gives:

(B-7) $$I_2 = \frac{15\pi^6}{32\ C_1^3\ (LMNP)^{3/2}} \left(\frac{a^4}{M^2} + \frac{b^4}{N^2} + \frac{c^4}{P^2} \right) + \frac{3\pi^6}{16\ C_1^3\ L^{3/2}(MNP)^{5/2}} \left(a^2b^2P + 5b^2c^2M + c^2a^2N \right)$$

(c)

(B-8) $$I_3 = \int e^{-\phi_2}\, R^2 R_2^2\, e^{-5\gamma R_{cm}^2}\, d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3\, d\vec{r}_4\, d\vec{r}_5$$

$$\vec{R}_2 = 1/3\ (\vec{r}_5 + \vec{r}_2 + \vec{r}_4) - \tfrac{1}{2}(\vec{r}_3 + \vec{r}_1)$$

$$\phi_2 = A_2(r_1^2 + r_3^2 + r_4^2 + r_5^2) + B_2 r_2^2 - \frac{B_2}{2}\ (\vec{r}_1 + \vec{r}_3 + \vec{r}_4 + \vec{r}_5)\cdot\vec{r}_2$$
$$+ 2C_2(\vec{r}_1 + \vec{r}_3)(\vec{r}_4 + \vec{r}_5) + 2D_2(\vec{r}_1\vec{r}_3 + \vec{r}_4\vec{r}_5)$$

A_2	$\frac{\alpha}{3} + \frac{\bar{\alpha}}{4} + \frac{13\beta}{60}$	$2.22 \times 10^{25}\ cm^{-2}$
B_2	$\frac{2\alpha}{3} + \frac{2\beta}{15}$	$1.93 \times 10^{25}\ cm^{-2}$
C_2	$-\frac{\beta}{5}$	$-0.0843 \times 10^{25}\ cm^{-2}$
D_2	$-\frac{\alpha}{6} - \frac{\bar{\alpha}}{4} + \frac{13\beta}{60}$	$-1.57 \times 10^{25}\ cm^{-2}$

Table II

Substituting the following change of variables in (B-8) :

$$\vec{\rho}_1 = \vec{r}_1 - \vec{r}_3$$
$$\vec{\rho}_2 = \vec{r}_4 - \vec{r}_5$$
$$\vec{\rho}_3 = \vec{r}_1 + \vec{r}_3 - \vec{r}_4 - \vec{r}_5$$
$$\vec{\rho}_4 = \tfrac{1}{4}(\vec{r}_1 + \vec{r}_3 + \vec{r}_4 + \vec{r}_5) - \vec{r}_2$$

I_3 becomes :

(B-9) $$I_3 = \frac{1}{8}\int exp\left(-L'\rho_1^2 - L'\rho_2^2 - M'\rho_3^2 - N'\rho_4^2\right)\left(a'\vec{\rho_3} + b'\vec{\rho_4}\right)^2 \times \left(-a'\vec{\rho_3} + b'\vec{\rho_4}\right)^2 \, d\vec{\rho_1}\, d\vec{\rho_2}\, d\vec{\rho_3}\, d\vec{\rho_4}$$

where: $L' = \frac{1}{2}(A_2 - D_2)$; $M' = \frac{B_2}{16} - C_2$; $N' = B_2$

$a' = 5/12$; $b' = -1/3$

Finally:

(B-10) $$I_3 = \frac{3\pi^6}{32\, L'^3 (M'N')^{7/2}} \left(5a'^4 N'^2 + 5b'^2 M'^2 + 2a'^2 b'^2 M'N'\right)$$

Numerically we have:

$I_1 = 2479.6 \times 10^{-200}\ cm^{16}$

$I_2 = 21.5 \times 10^{-200}\ cm^{16}$

$I_3 = 203.6 \times 10^{-200}\ cm^{16}$

Hence, from equation (B-1), we deduce:

(B-11) $$N_i^2 = \frac{8}{I_1 - 2I_2 + I_3} = 3.03 \times 10^{197}\ cm^{-16}$$

2.- Evaluation of N_f.

Let:

$I_4 = \left\langle (1234;5) \middle| (1234;5) \right\rangle_{m_L=1}$

$I_5 = \left\langle (1234;5) \middle| (5234;1) \right\rangle_{m_L=1}$

or:

$$I_4 = \int exp\left(-\frac{\alpha_1}{12}\rho_1^2 - \frac{\alpha_1}{6}\rho_2^2 - \frac{\alpha_1}{2}\rho_3^2 - \frac{4\beta'}{5}R_1^2\right) R_1^2\, Y_1^1(\Omega_1)\, Y_1^{1*}(\Omega_1) \times e^{-5\gamma R_{cm}^2}\, d\vec{r_1}\, d\vec{r_2}\, d\vec{r_3}\, d\vec{r_4}\, d\vec{r_5}$$

where:

$$\vec{\rho}_1 = 3\vec{r}_1 - (\vec{r}_2 + \vec{r}_3 + \vec{r}_4)$$
$$\vec{\rho}_2 = 2\vec{r}_2 - (\vec{r}_3 + \vec{r}_4)$$
$$\vec{\rho}_3 = \vec{r}_3 - \vec{r}_4$$
$$\vec{R}_1 = \tfrac{1}{4}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_5$$

(B-12) $$I_4 = \frac{3 \times 5^{5/2} \pi^5}{2^5 \beta'^{5/2} \alpha_1^{9/2}}$$

and:

(B-13) $$I_5 = \int e^{-\phi} R_1 R_2 \mathcal{Y}_1^{1*}(\Omega_1) \mathcal{Y}_1^1(\Omega_2) e^{-5\gamma R_{cm}^2} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

where:

$$\vec{R}_2 = \tfrac{1}{4}(\vec{r}_5 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_1$$

$$\phi = A(r_2^2 + r_3^2 + r_4^2) + B(r_1^2 + r_5^2) + 2C(\vec{r}_2\vec{r}_3 + \vec{r}_3\vec{r}_4 + \vec{r}_4\vec{r}_2)$$
$$+ 2D(\vec{r}_1 + \vec{r}_5)(\vec{r}_2 + \vec{r}_3 + \vec{r}_4) + 2E\vec{r}_1\vec{r}_5$$

A	$\frac{3\alpha_1}{4} + \frac{\beta'}{20}$	3.36×10^{25} cm^{-2}	3.41×10^{25} cm^{-2}
B	$\frac{3\alpha_1}{8} + \frac{17\beta'}{40}$	2.58×10^{25} cm^{-2}	3.00×10^{25} cm^{-2}
C	$-\frac{\alpha_1}{4} + \frac{\beta'}{20}$	-0.97×10^{25} cm^{-2}	-0.92×10^{25} cm^{-2}
D	$-\frac{\alpha_1}{8} - \frac{3\beta'}{40}$	-0.71×10^{25} cm^{-2}	-0.79×10^{25} cm^{-2}
E	$-\frac{\beta'}{5}$	-0.45×10^{25} cm^{-2}	-0.65×10^{25} cm^{-2}

Table III

Coefficients A,B, . . . E are given in Table III. Here, we have two sets of numerical values for these coefficients since two possible values of β' are given by Pearlstein, Tang and Wildermuth (6).

ϕ can be written as :

$$\phi = L\rho_1^2 + M\rho_2^2 + N\rho_3^2 + P\rho_4^2$$

where: $L = \frac{1}{A}$; $M = \frac{A-C}{A(A+C)}$; $N = \frac{D(C-A)}{2(A+C)}$; $P = -\frac{1}{4}(3C+7E)$

and:

$$\vec{\rho}_1 = A\vec{r}_2 + C(\vec{r}_3 + \vec{r}_4) + D(\vec{r}_1 + \vec{r}_5)$$
$$\vec{\rho}_2 = (A+C)\vec{r}_3 + C\vec{r}_4 + D(\vec{r}_1 + \vec{r}_5)$$
$$\vec{\rho}_3 = \vec{r}_1 + \vec{r}_5 - 2\vec{r}_4$$
$$\vec{\rho}_4 = \vec{r}_1 - \vec{r}_5$$

In terms of the new variables, (B-13) becomes:

$$I_5 = \frac{1}{8A^3(A+C)^3}\int exp\left(-L\rho_1^2 - M\rho_2^2 - N\rho_3^2 - P\rho_4^2\right)\times\Big(a\rho_1 Y_1^{1*}(\Omega_1) + b\rho_2 Y_1^{1*}(\Omega_2) + c\rho_3 Y_1^{1*}(\Omega_3) + d\rho_4 Y_1^{1*}(\Omega_4)\Big)\Big(a\rho_1 Y_1^{1}(\Omega_1) + b\rho_2 Y_1^{1}(\Omega_2) + c\rho_3 Y_1^{1}(\Omega_3) - d\rho_4 Y_1^{1}(\Omega_4)\Big)\, d\vec{\rho}_1\, d\vec{\rho}_2\, d\vec{\rho}_3\, d\vec{\rho}_4$$

$$I_5 = \frac{1}{8A^3(A+C)^3}\left(\frac{a^2}{L} + \frac{b^2}{M} + \frac{c^2}{N} - \frac{d^2}{P}\right)\frac{3\pi^5}{8(LMNP)^{3/2}}$$

where: $a = \frac{1}{4A}$; $b = \frac{A-C}{4A(A+C)}$; $c = \frac{C-A}{8(A+C)}$; $d = 5/8$

Numerically, we have two sets of values of I_4 and I_5 and two possible values of N_f :

1) $I_4 = 2.866 \times 10^{-176} \text{ cm}^{14}$

$I_5 = -0.560 \times 10^{-176} \text{ cm}^{14}$

$$N_f^2 = \frac{12}{I_4 - I_5} = 3.50 \times 10^{176} \text{ cm}^{-14}$$

2) $I_4 = 1.147 \times 10^{-176} \text{ cm}^{14}$

$I_5 = -0.273 \times 10^{-176} \text{ cm}^{14}$

$$N_f^2 = \frac{12}{I_4 - I_5} = 8.45 \times 10^{176} \text{ cm}^{-14}$$

APPENDIX C

REDUCTION OF CERTAIN QUADRATIC FORMS

The object of this appendix is to reduce the following quadratic forms:

$$\phi = A(r_1^2 + r_2^2 + r_3^2) + Br_4^2 + Cr_5^2 + 2D(r_1r_2 + r_2r_3 + r_3r_1) + 2(Er_4 + Fr_5)(r_1 + r_2 + r_3) + 2Gr_4r_5 \tag{C-1}$$

and:

$$\phi' = A'r_1^2 + B'(r_2^2 + r_3^2) + C'(r_4^2 + r_5^2) + 2r_1\left[D'(r_2 + r_3) + E'(r_4 + r_5)\right] + 2F'r_2r_3 + 2G'r_4r_5 + 2H'(r_2 + r_3)(r_4 + r_5) \tag{C-2}$$

to sums of four square terms.

As an example, we choose to perform the reduction of the quadratic form ϕ'. The result of the reduction of ϕ will also be given.

In order to evaluate the integral B_k (equation IV-23) :

$$B_k = \left\langle (5234;1)_k \middle| \bar{r}_3 Y_1^k(\bar{\omega}_3) + \bar{r}_4 Y_1^k(\bar{\omega}_4) \middle| (123;45) \right\rangle$$
$$= \int e^{-\phi'} R_1' \, \mathcal{Y}_1^{k*}(\Omega_1') \, R^2 \left(\vec{r}_3 \, \mathcal{Y}_1^k(\bar{\omega}_3) + \vec{r}_4 \, \mathcal{Y}_1^k(\bar{\omega}_4) \right) e^{-5\gamma R_{cm}^2} \, d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

we shall find a linear transformation from the variables $(r_1, r_2, r_3, r_4, r_5)$ (in fact, we must write $\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{r}_5$ for these variables are vectors, but we adopt these simplified notations in this appendix without confusion) to the new variables (s_1,s_2,s_3,s_4,s_5) , such that :

(a) $\phi' = ls_1^2 + ms_2^2 + ns_3^2 + ps_4^2 + qs_5^2$

Note that it is not necessary that all coefficients l,m,n,p,q be different from zero; we shall see later that one of them is in fact zero.

(b) One of the new variable, say $s_1 \propto R_1'$

or: $s_1 \propto \frac{r_2+r_3+r_4+r_5}{4} - r_1$

In Table I, the coefficients A',B',C', . . . of the form ϕ' are expressed in terms of the width parameters α , α_1 , $\bar{\alpha}$, β and β'.

A'	$\frac{\alpha}{3} + \frac{\beta}{15} + \frac{2\beta'}{5}$	E'	$-\frac{\beta}{10} - \frac{\beta'}{10}$
B'	$\frac{\alpha}{3} + \frac{3\alpha_1}{8} + \frac{\beta}{15} + \frac{\beta'}{40}$	F'	$-\frac{\alpha}{6} - \frac{\alpha_1}{8} + \frac{\beta}{15} + \frac{\beta'}{40}$
C'	$\frac{3\alpha_1}{8} + \frac{\bar{\alpha}}{4} + \frac{3\beta}{20} + \frac{\beta'}{40}$	G'	$-\frac{\alpha_1}{8} - \frac{\bar{\alpha}}{4} + \frac{3\beta}{20} + \frac{\beta'}{40}$
D'	$-\frac{\alpha}{6} + \frac{\beta}{15} - \frac{\beta'}{10}$	H'	$-\frac{\alpha_1}{8} - \frac{\beta}{10} + \frac{\beta'}{40}$

Table I

In what follows, the theory of the reduction of a quadratic form to a sum of square terms is quoted briefly. A more detailed theory can be found in reference (10).

First, we consider the quadratic form ϕ' as a scalar function of the vector $\vec{V} = (r_1,r_2,r_3,r_4,r_5)$:

$$\phi' = \phi'(\vec{V})$$

Then, we define the polar form φ associated with the quadratic form ϕ' :

$$\text{(C-3)} \qquad \varphi(\vec{V},\vec{W}) = \tfrac{1}{2}\sum_{i=1}^{5} t_i \frac{\partial \phi'}{\partial r_i}$$

$$\begin{aligned}
&= t_1\Big(A' r_1 + D'(r_2+r_3) + E'(r_4+r_5)\Big) \\
&+ t_2\Big(B' r_2 + D' r_1 + F' r_3 + H'(r_4+r_5)\Big) \\
&+ t_3\Big(B' r_3 + D' r_1 + F' r_2 + H'(r_4+r_5)\Big) \\
&+ t_4\Big(C' r_4 + E' r_1 + G' r_5 + H'(r_2+r_3)\Big) \\
&+ t_5\Big(C' r_5 + E' r_1 + G' r_4 + H'(r_2+r_3)\Big)
\end{aligned}$$

where $\vec{W} = (t_1, t_2, t_3, t_4, t_5)$

From this definition and from the equation:

$$\vec{V} = \sum_{i=1}^{5} r_i \vec{e}_i$$

(where $\{\vec{e}_i\}$ are vectors of a basis in which the quadratic form ϕ' has the form (C-2)) an important relation can be deduced :

$$\text{(C-4)} \qquad \phi'(\vec{V}) = \varphi(\vec{V},\vec{V}) = \sum_{i=1}^{5}\sum_{j=1}^{5} r_i r_j \varphi(\vec{e}_i, \vec{e}_j)$$

If we change to a new basis $\{\vec{\mathcal{E}}_j\}$, the new components of $\vec{V}$ will be s_1, s_2, s_3, s_4, s_5 so that :

$$\vec{V} = \sum_{j=1}^{5} s_j \vec{\mathcal{E}}_j$$

Equation (C-4) becomes therefore:

$$\text{(C-5)} \qquad \phi'(V) = \sum_{i=1}^{5}\sum_{j=1}^{5} s_i s_j \varphi(\vec{\mathcal{E}}_i, \vec{\mathcal{E}}_j)$$

From this equation, we can see that if the transformation of the old basis $\{\vec{e}_i\}$ to the new basis $\{\vec{\mathcal{E}}_j\}$ is chosen such that:

(C-6) $$\varphi(\vec{\mathcal{E}}_i,\vec{\mathcal{E}}_j) = 0 \quad \text{for} \quad i \neq j$$

all cross terms in (C-5) will vanish, that is ;

$$\phi'(\vec{V}) = \sum_{i=1}^{5} \varphi(\vec{\mathcal{E}}_i,\vec{\mathcal{E}}_i)\, s_i^2$$

or:

(C-7) $$\phi'(\vec{V}) = \sum_{i=1}^{5} \phi'(\vec{\mathcal{E}}_i)\, s_i^2$$

In matrix equations, the linear transformation of the new basis to the old basis, and that of the old variables to the new variables can be written respectively as follows:

(C-8) $$\begin{bmatrix} \vec{e}_1 \\ \vec{e}_2 \\ \vec{e}_3 \\ \vec{e}_4 \\ \vec{e}_5 \end{bmatrix} = T \begin{bmatrix} \vec{\mathcal{E}}_1 \\ \vec{\mathcal{E}}_2 \\ \vec{\mathcal{E}}_3 \\ \vec{\mathcal{E}}_4 \\ \vec{\mathcal{E}}_5 \end{bmatrix}$$

(C-9) $$\begin{bmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \\ s_5 \end{bmatrix} = \widetilde{T} \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \end{bmatrix}$$

where T is a 5×5 matrix and $\widetilde{T}$ its transpose.

The choice of T such that equation (C-6) (and consequently, condition (a)) and condition (b) are satisfied is not unique. One particular choice can be obtained in the following way: $\vec{\mathcal{E}}_1$ can be chosen as a linear function of the $\vec{e}_i$'s arbitrarily (for instance we choose $\vec{\mathcal{E}}_1 = \vec{e}_1$, that is, in the equation $\vec{\mathcal{E}}_1 = \sum_{i=1}^{5} x_i e_i$, we put $x_1=1$, $x_2 = x_3 = x_4 = x_5 = 0$, because we have five independent variables). Now, with this vector $\vec{\mathcal{E}}_1$, the second vector $\vec{\mathcal{E}}_2$ can be chosen with the condition that : $\varphi(\vec{\mathcal{E}}_1,\vec{\mathcal{E}}_2)=0$, so that the choice of $\vec{\mathcal{E}}_2$ is less arbitrary than that of $\vec{\mathcal{E}}_1$:we have only four independent variables. The third vector $\vec{\mathcal{E}}_3$ must satisfy simultaneously : $\varphi(\vec{\mathcal{E}}_1,\vec{\mathcal{E}}_3)=\varphi(\vec{\mathcal{E}}_2,\vec{\mathcal{E}}_3)=0$, and so on . . . . In this way, $\vec{\mathcal{E}}_1, \vec{\mathcal{E}}_2 \dots \vec{\mathcal{E}}_5$ are selected in terms of $\{\vec{e}_i\}$ such a manner that all equations $\varphi(\vec{\mathcal{E}}_i,\vec{\mathcal{E}}_j)=0$ $(i \neq j)$ are satisfied.

The fact that one of the new variables s_1 is determined beforehand (in condition (b)) complicates the choice of T but does not restrict it to be a unique choice.

After a tedious calculation,we find that:

$$\text{(C-10)} \qquad \begin{bmatrix} \vec{\mathcal{E}}_1 \\ \vec{\mathcal{E}}_2 \\ \vec{\mathcal{E}}_3 \\ \vec{\mathcal{E}}_4 \\ \vec{\mathcal{E}}_5 \end{bmatrix} = \begin{bmatrix} 0 & -\lambda & -\lambda & \frac{1}{2}+\lambda & \frac{1}{2}+\lambda \\ 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & 1 & -1 & -1 \end{bmatrix} \begin{bmatrix} \vec{e}_1 \\ \vec{e}_2 \\ \vec{e}_3 \\ \vec{e}_4 \\ \vec{e}_5 \end{bmatrix}$$

where:

$$\lambda = \frac{2H' - (C' + G')}{2(B' + C' + F' + G' - 4H')}$$

The 5×5 matrix in (C-10) is just T^{-1} ; hence:

$$\text{(C-11)} \quad \begin{bmatrix} \vec{e}_1 \\ \vec{e}_2 \\ \vec{e}_3 \\ \vec{e}_4 \\ \vec{e}_5 \end{bmatrix} = \begin{bmatrix} -4 & 1 & 0 & 0 & -(4\lambda+1) \\ 1 & 0 & 0 & \frac{1}{2} & \lambda+\frac{1}{2} \\ 1 & 0 & 0 & -\frac{1}{2} & \lambda+\frac{1}{2} \\ 1 & 0 & \frac{1}{2} & 0 & \lambda \\ 1 & 0 & -\frac{1}{2} & 0 & \lambda \end{bmatrix} \begin{bmatrix} \vec{\varepsilon}_1 \\ \vec{\varepsilon}_2 \\ \vec{\varepsilon}_3 \\ \vec{\varepsilon}_4 \\ \vec{\varepsilon}_5 \end{bmatrix}$$

From this equation, it follows that :

$$\text{(C-12)} \quad \begin{bmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \\ s_5 \end{bmatrix} = \begin{bmatrix} -4 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 & 0 \\ -(4\lambda+1) & \lambda+\frac{1}{2} & \lambda+\frac{1}{2} & \lambda & \lambda \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \end{bmatrix}$$

Using (C-7), ϕ' can be now written as :

$$\text{(C-13)} \quad \phi' = \phi'(\vec{\varepsilon}_1)\,(r_2+r_3+r_4+r_5-4r_1)^2 + \phi'(\vec{\varepsilon}_2)\,r_1^2 + \phi'(\vec{\varepsilon}_3)\left(\frac{r_4-r_5}{2}\right)^2$$
$$+\phi'(\vec{\varepsilon}_4)\left(\frac{r_3-r_2}{2}\right)^2 + \phi'(\vec{\varepsilon}_5)\Big[-(4\lambda+1)r_1+(\lambda+\tfrac{1}{2})(r_2+r_3)$$
$$+\lambda(r_4+r_5)\Big]^2$$

where $\phi'(\vec{\varepsilon}_i)$ can be evaluated by expressing the $\vec{\varepsilon}_i$ as functions of the old basis vectors $\vec{e}_j$ (see equation C-10) , and substituting these expressions into (C-2) :

$$\phi'(\vec{\varepsilon}_1) = \tfrac{1}{2}(C' + G') - \lambda(E' + 4H') \quad ; \quad \phi'(\vec{\varepsilon}_2) = 0$$

$$\phi'(\vec{\varepsilon}_3) = 2(C' - G') \quad ; \quad \phi'(\vec{\varepsilon}_4) = 2(B' - F')$$

$$\phi'(\vec{\varepsilon}_5) = 2(B' + C' + F' + G' - 4H') .$$

Finally, changing notation, ϕ' becomes :

$$\phi' = L'\rho_1^2 + M'\rho_2^2 + N'\rho_3^2 + P'\rho_4^2 \tag{C-14}$$

where:

$$\begin{cases} \rho_1 = \tfrac{1}{4}(r_2 + r_3 + r_4 + r_5) - r_1 \\ \rho_2 = r_4 - r_5 \\ \rho_3 = r_2 - r_3 \\ \rho_4 = X'r_1 + Y'(r_2 + r_3) + Z'(r_4 + r_5) \end{cases}$$

In Table II, L', M', N', P', X', Y' and Z' are expressed in terms of A', B', . . . H'.

L'	$8(C'+G') - \dfrac{8(E'+4H')^2}{B'+C'+F'+G'-4H'}$
M'	$\tfrac{1}{2}(C'-G')$
N'	$\tfrac{1}{2}(B'-F')$
P'	$\tfrac{1}{2}(B'+C'+F'+G'-4H')^{-1}$
X'	$2(D'-E')$
Y'	$-(D'+4H')$
Z'	$E'+4H'$

Table II

We turn now to the quadratic form ϕ . Table III gives the coefficients of ϕ in terms of the width parameters α, α_1, $\bar{\alpha}$, β and β'.

A	$\frac{\alpha}{3} + \frac{3\alpha_1}{8} + \frac{\beta}{15} + \frac{\beta'}{40}$	E	$-\frac{\alpha_1}{8} - \frac{\beta}{10} + \frac{\beta'}{40}$
B	$\frac{3\alpha_1}{8} + \frac{\bar{\alpha}}{4} + \frac{3\beta}{20} + \frac{\beta'}{40}$	B	$-\frac{\beta}{10} - \frac{\beta'}{10}$
C	$\frac{\bar{\alpha}}{4} + \frac{3\beta}{20} + \frac{2\beta'}{5}$	G	$-\frac{\bar{\alpha}}{4} + \frac{3\beta}{20} - \frac{\beta'}{10}$
D	$-\frac{\alpha}{6} - \frac{\alpha_1}{8} + \frac{\beta}{15} + \frac{\beta'}{40}$		

Table III

The reduction of ϕ can be performed in a similar way :

(C-16) $$\phi = L\rho_1^2 + M\rho_2^2 + \rho_3^2 + \rho_4^2$$

where:

(C-17) $$\begin{cases} \rho_1 = \frac{1}{4}(r_1 + r_2 + r_3 + r_4) - r_5 = R_1 \\ \rho_2 = r_1 - r_2 \\ \rho_3 = X(r_1 + r_2 + r_3) + Yr_4 + Zr_5 \\ \rho_4 = S(r_1 + r_2 - 2r_3) \end{cases}$$

and the coefficients L,M,X,Y,Z, and S are given in Table IV (page 57)

L	$-\frac{16}{3}(E+F) - \frac{16(4E+F)^2}{16B+8G+C}$
M	$\frac{1}{2}(A-D)$
X	$\frac{4E+F}{(16B+8G+C)^{\frac{1}{2}}}$
Y	$\frac{4B+G}{(16B+8G+C)^{\frac{1}{2}}}$
Z	$\frac{4G+C}{(16B+8G+C)^{\frac{1}{2}}}$
S	$\left(\frac{A+D}{2} + \frac{E+F}{3}\right)^{\frac{1}{2}}$

Table IV

BIBLIOGRAPHY AND CITED REFERENCES

1) K. Wildermuth and Th. Kanellopoulos, CERN Report 59-23

2) K. Wildermuth, Lectures on the cluster model of the nucleus. Physics Dept. Technical Report No.281.University of Maryland.

3) K. Wildermuth and Th. Kanellopoulos, Nuclear Phys. 14, 349 (1959-60).

4) A. Messiah, Mécanique Quantique vol.II (Chapter XIV) Dunod (Paris).

5) G.Derrick and J.M. Blatt, Nuclear Phys. 8 , 310 (1958)

6) L.D. Pearlstein,Y.C. Tang,K. Wildermuth, Phys.Rev.120, 224 (1960).

7) M.A. Preston, Physics of the nucleus (Ch.XI) ,Addison-Wesley (1962)

8) K. Siegbahn, Alpha, beta and gamma-ray spectroscopy vol.2 (Ch.XV), North-Holland Publishing Co.(1965)

9) J.M. Blatt and V.F. Weisskopf, Theoretical nuclear physics (Ch.XII), Wiley(1952)

10) A.Lentin and J.Rivaud, Eléments d'algèbre moderne (pp. 228-239), Vuibert-Paris (1958).

11) J.M. Blair, N.M.Hintz, D.M.Van Patter, Phys.Rev. 96,1023(1954)

12) G.A. Sawyer and L.C. Burkhardt, Phys.Rev. 98,1305 (1955)

13) J.H. Coon and R.W. Davis, Bull.Am. Phys. Soc. 4,366 (1959).

14) H.A. Bethe and E.E. Salpeter, Quantum mechanics of one- and two-electron atoms (p.251), Academic Press inc. New York (1957).