

ALTERNATIVE METHOD FOR
CALCULATION OF THE RADIATIVE WIDTH OF
THE $\frac{3}{2}^+$ STATE IN He^5 USING THE CLUSTER MODEL

by

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ABSTRACT

An alternative form of the electric dipole transition operator which can test the correctness of wave functions at small distances from the centre of mass of the nucleus is derived to calculate the level width of the $3/2 +$ state in He^5 nucleus using cluster model wave functions.

The result is found to be two times larger than the experimental value. This indicates that the cluster model wave functions are not very good at small distances. It is shown that the large calculated value for the level width may result from the fact that the effect of the hard core of the nuclear force is not taken into account in the cluster model wave functions.

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CHAPTER I

INTRODUCTION

In the last few decades, a number of nuclear models and theories have been developed in order to explain the behaviour of the nucleus. Although they have been partially successful in fitting a large quantity of experimental data, none is able to explain the properties of the nucleus as a whole. There does not yet exist a well established unified theory of the nucleus such as exists in the case of the atom. The main difficulty lies in the fact that the nuclear force is not completely known. However, the various nuclear models are helpful in correlating the behaviour of the nucleus.

From various measurable properties of the nucleus, both collective and individual particle features can be seen. The models which reflect the properties of these two extreme cases are the liquid droplet model and the single particle model. The liquid droplet model predicts the binding energy, instability toward fission and β -decay, nuclear radius and other properties, while the single particle model is quite successful in predicting energy levels, magic numbers and spins. However, in some nuclei, particularly light nuclei, the theoretical values of the energy levels of some excited states calculated from the single particle model are not in good agreement with the experimental values. There is evidence that the nucleons group together to form clusters. The nucleons within a cluster are bound

more tightly together than to the others, and show collective features. The cluster model is based essentially on this evidence, and is appropriate to describe many phenomena in light nuclei^{(1)*}.

1. The He⁵ Nucleus

We shall use He⁵ as an example to review briefly the formulation of the cluster model.

The He⁵ nucleus is composed of three neutrons and two protons. The ground state of this nucleus has total angular momentum 3/2 with odd parity. In the single particle model (see Fig.1-1), two neutrons and two protons occupy the 1s level, and one neutron is in the 1p level. The 1s nucleons couple to give zero spin, and the 1p neutron has $s=\frac{1}{2}$, $l=1$ with a resultant $j=3/2$. Since in the single particle model, all nucleons are assumed to move in a simple harmonic oscillator potential, calculations show that the 1p neutron has energy $\hbar\omega$ relative to the 1s level. In the cluster model, we look upon the 1s nucleons as an α -particle cluster which is tightly bound, so that the outside neutron moves relative to the α -particle in a simple harmonic potential with energy $\hbar\omega$. Since the α -particle has large binding energy, it is unlikely that it has internal excitation in the ground state.

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

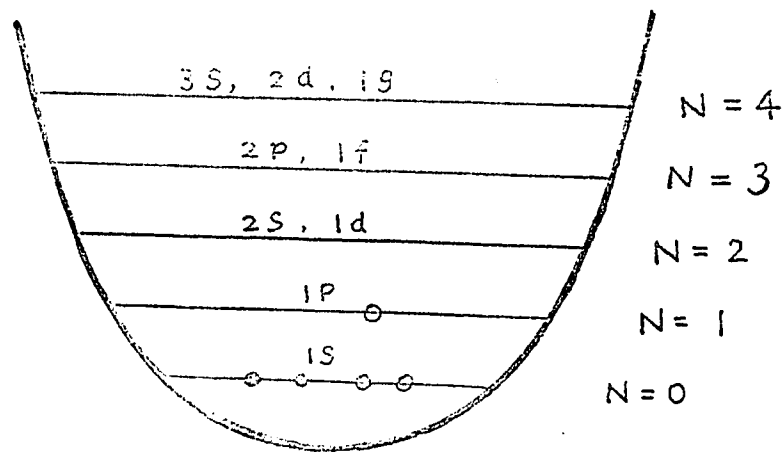


Fig. 1-1 The single particle model for the $3/2^-$ state of the He^5 nucleus. \circ denotes neutrons and \odot denotes protons.

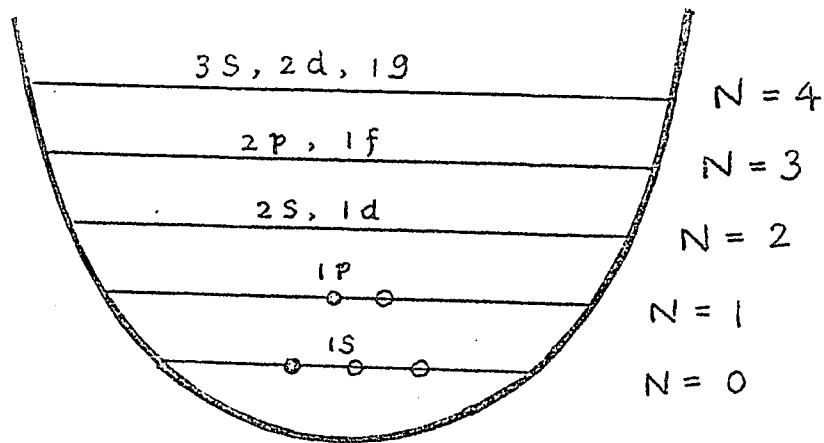


Fig. 1-2 The single particle model for the $3/2^+$ state of the He^5 nucleus. \circ denotes neutrons and \odot denotes protons.

Therefore, the spatial part of the ground state wave function can be written as

$$\Psi\left(\frac{3}{2}^-\right) = \varphi(\alpha)\varphi(n) \chi(\vec{R}_\alpha - \vec{R}_n) W(\vec{R}_{cm}) \quad (1-1)$$

where $\varphi(\alpha)$, $\varphi(n)$ denote the α -particle and neutron wave functions respectively, $\chi(\vec{R}_\alpha - \vec{R}_n)$ represents the relative motion between them, and $W(\vec{R}_{cm})$ is the wave function of the centre of mass.

The solution of the Schrodinger equation of the three-dimensional harmonic oscillator is

$$\Psi_{n,l,m} = N e^{-\frac{r^2}{2}} r^l L_k^{l+\frac{1}{2}}(r^2) Y_l^m(\theta, \phi) \quad (1-2)$$

where N is a normalization constant, $L_k^{l+\frac{1}{2}}$ is a Laguerre polynomial, Y_l^m is a spherical harmonic and r is measured in units of $(\hbar/m\omega)^{\frac{1}{2}}$ with $\omega^2 = K/m$, K being the force constant. l specifies the orbital angular momentum and $k = \frac{1}{2}(n-1)$, where n is the principal quantum number, related to the energy by

$$E_n = (n + 3/2)\hbar\omega$$

The orbital angular momentum of the nucleons in the α cluster is assumed to be zero in the ground state, i.e. $l=0$. For the neutron outside the α cluster, $l=1$, $n=1$ and hence $k=0$. Therefore, eq.(1-1) can be written as

$$\Psi\left(\frac{3}{2}^-\right) = N \exp\left(-\frac{\alpha}{2} \sum_{i=1}^4 r_i'^2\right) R_1 Y_1^m(\Omega_1) e^{-\frac{2\beta'}{5} R_1^2} e^{-\frac{5\gamma}{2} R_{cm}^2} \quad (1-3)$$

where

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

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

$$\vec{R}_1 = \vec{R}_\alpha - \vec{r}_5 \quad (1-4)$$

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

If the same force constants were used in $\varphi(n)$ and $\chi(\vec{R}_\alpha - \vec{R}_n)$, the cluster model wave function would be exactly equivalent to the single particle model wave function, and no cluster correlations would be included. In order to get a wave function close to the exact one, α , and β' must be treated as parameters and a variational method used to determine their values. This has been done by Pearlstein et al (2)

The $3/2+$ excited state of He^5 at 16.7 Mev. can be described in the single particle model as a single proton excitation to the $1p$ state (see Fig. 1-2). This gives a system with two quanta of energy $2\hbar\omega$, so that in the cluster model wave function, the relative motion of the two clusters must be described by a function having two quanta of oscillation. It has been shown by Pearlstein et al. (2) that the alpha-neutron configuration does not give a minimum as a result of variational calculation with respect to width parameters. We therefore have to use the deuteron-triton picture for the $3/2+$ state. This configuration also accounts for the well known resonance in the deuteron-triton scattering cross-section.

The wave function for the $3/2+$ state is then

$$\varphi(\frac{3}{2}+) = \varphi(t) \varphi(d) \chi(\vec{R}_t - \vec{R}_d) W(R_{cm}) \quad (1-5)$$

In this state, $n=2$ and $l=0$, so that $k=1$ in eq.(1-2).

The triton and deuteron are assumed to be in their ground states. With

$$L_1^{\frac{1}{2}} = 3/2 - r^2 \quad (1-6)$$

the wave function of the $3/2 +$ state can be written explicitly in the following form

$$\begin{aligned} \Psi\left(\frac{3}{2} +\right) = \exp\left(-\frac{\alpha}{2} \sum_{i=1}^3 r_i'^2 - \frac{\bar{\alpha}}{2} \sum_{j=4}^5 r_j'^2\right) \\ R^2 Y_0^0(\Omega) \exp\left(-\frac{3\beta}{5} R^2\right) \exp\left(-\frac{5\gamma}{2} R_{cm}^2\right) \quad (1-7) \end{aligned}$$

where

$$\begin{aligned} \vec{r}_i' &= \vec{r}_i - \vec{R}_t & (i = 1, 2, 3) \\ \vec{r}_j' &= \vec{r}_j - \vec{R}_d & (j = 4, 5) \\ \vec{R}_t &= 1/3 (\vec{r}_1 + \vec{r}_2 + \vec{r}_3) \\ \vec{R}_d &= 1/2 (\vec{r}_4 + \vec{r}_5) \\ \vec{R} &= \vec{R}_t - \vec{R}_d \end{aligned} \quad (1-8)$$

The first term in eq.(1-6) vanishes under antisymmetrization.

Again the parameters α, β and $\bar{\alpha}$ are determined by the variational method (2). The factors in eqs.(1-3) and (1-7) corresponding to the motion of the centre of mass will be dropped in the calculation, since the harmonic oscillator potential is fixed in space and not invariant to the transformation to the centre of mass system.

2. Antisymmetrized Wave Functions (3)

A complete wave function to describe a nuclear system must include both spatial and spin wave functions. Furthermore, since protons and neutrons are fermions, the wave function must be antisymmetric with respect to exchange of the spatial and spin coordinates of two identical particles.

In this work, proton and neutron are looked upon as distinct particles, so that the isotopic spin formalism need not be used.

The complete antisymmetrized wave functions of the ground state have been found by Tran Duc ⁽³⁾, and their explicit forms are given in Appendix A.

In the calculation of the transition probability, only unantisymmetrized wave functions of the excited state with $M_J = \pm \frac{1}{2}$ are used. They are found to be ⁽³⁾

$$\begin{aligned} \varphi_i\left(\frac{1}{2}\right) = \frac{N_i}{\sqrt{18}} & \left[(\alpha_1\beta_3 + \beta_1\alpha_3)(\alpha_2\alpha_4\beta_5 + \alpha_2\beta_4\alpha_5 \right. \\ & \left. + \beta_2\alpha_4\alpha_5) - 2\alpha_1\beta_2\alpha_3(\alpha_4\beta_5 + \beta_4\alpha_5) \right. \\ & \left. - 2\beta_1\alpha_2\beta_3\alpha_4\alpha_5 \right] (123;45) \end{aligned} \quad (1-9)$$

$$\begin{aligned} \varphi_i\left(-\frac{1}{2}\right) = \frac{N_i}{\sqrt{18}} & \left[(\alpha_1\beta_3 + \beta_1\alpha_3)(\alpha_2\beta_4\beta_5 + \beta_2\alpha_4\beta_5 \right. \\ & \left. + \beta_2\beta_4\alpha_5) - 2\beta_1\alpha_2\beta_3(\alpha_4\beta_5 + \beta_4\alpha_5) \right. \\ & \left. - 2\alpha_1\beta_2\alpha_3\beta_4\beta_5 \right] (123;45) \end{aligned} \quad (1-10)$$

where N_i is a normalization constant.

The notations are the same as those used by Tran Duc. (123;45) and (1234;5) represent the spatial wave functions of the excited state and the ground state respectively; the first two and fifth positions denote neutrons; the third and fourth positions denote protons; the numbers denote different particles. α_k denotes the particle k with $m_s = \frac{1}{2}$, while β_k denotes the particle k with $m_s = -\frac{1}{2}$.

3. Radiative Transition Probability ⁽³⁾(4)

The $3/2 +$ excited state of the He^5 nucleus is unstable

to gamma decay to the $3/2$ - ground state (see Fig.1-3). The level width has been determined experimentally to be of order 1.32 ev ⁽⁵⁾. Using the wave functions in the previous section, it is possible to calculate theoretically the transition probability of this transition.

The transition is from the initial state $J_i = 3/2$ to the final state $J_f = 3/2$ with parity change. Therefore, according to the selection rules of multipole radiation ⁽⁶⁾, the only allowed transitions are $l = 1, 3$ for electric radiation and $l = 2$ for magnetic radiation, where l is the quantum number specifying the angular momentum of the emitted photon. Contribution due to $l = 2, 3$ transitions are small compared to $l = 1$ transition and can be neglected.

The expression for transition probability of E1 transition is shown to be ⁽³⁾⁽⁷⁾

$$T_E(1) = \frac{4\pi e^2 k^3}{9 \hbar} \sum_{M_i, M_f} |\langle f | R_{1m} | i \rangle|^2 \quad (1-11)$$

where $R_{1m} = \sum_i \bar{r}_i Y_1^m(\Omega_i)$ (1-12)

the summation being over all protons, and \bar{r}_i being the coordinate in the centre of mass system.

By the selection rule and the orthogonality property of the spin coordinates, it can be shown ⁽³⁾ that the summation on the right hand side of eq.(1-11) is

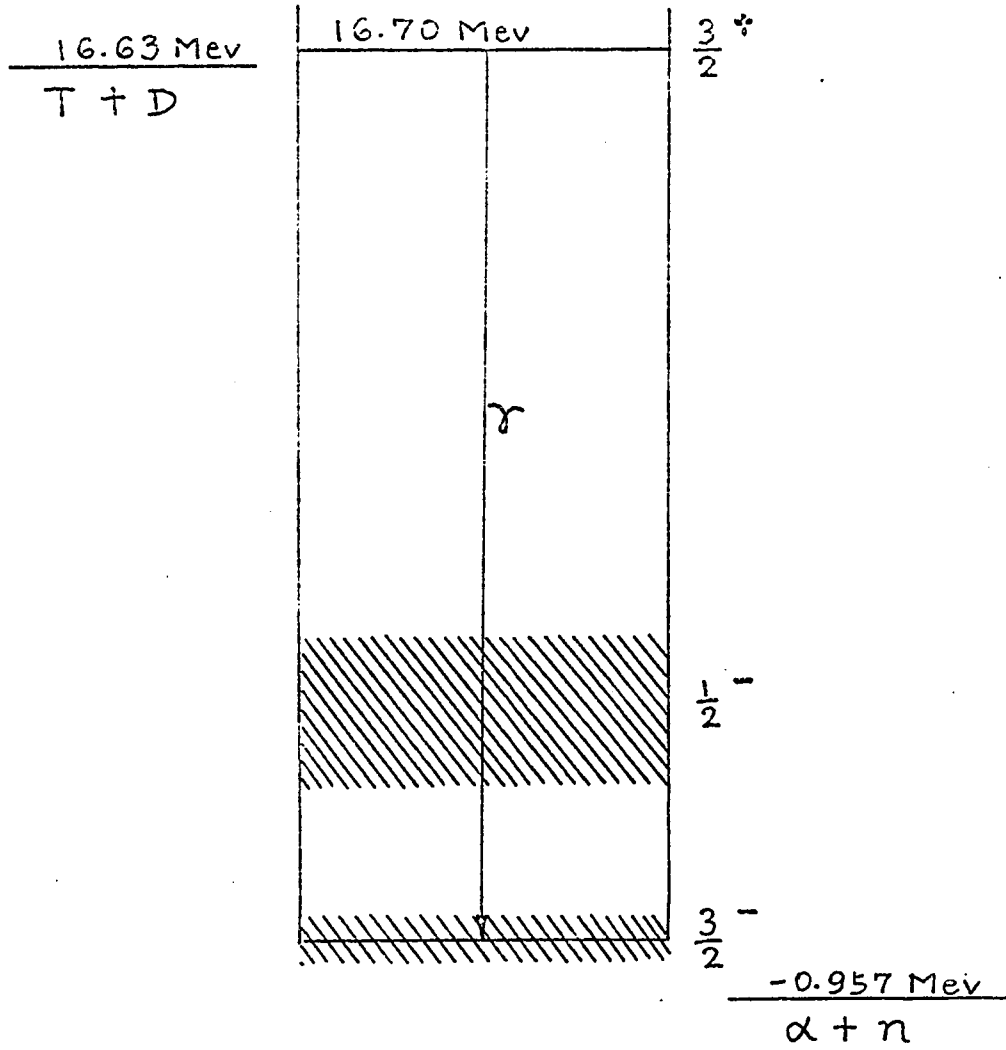


Fig.1-3. Energy level diagram for the He^5 nucleus.

$$\begin{aligned}
 B_E(1) &= \sum_{M_i, M_f} |\langle f | R_{1m} | i \rangle|^2 \\
 &= |\langle \bar{\Phi}_f(\frac{3}{2}) | R_{1-1} | \bar{\Phi}_i(\frac{1}{2}) \rangle|^2 + |\langle \bar{\Phi}_f(\frac{1}{2}) | R_{10} | \bar{\Phi}_i(\frac{1}{2}) \rangle|^2 \\
 &\quad + |\langle \bar{\Phi}_f(\frac{1}{2}) | R_{1-1} | \bar{\Phi}_i(-\frac{1}{2}) \rangle|^2 + |\langle \bar{\Phi}_f(-\frac{1}{2}) | R_{11} | \bar{\Phi}_i(\frac{1}{2}) \rangle|^2 \\
 &\quad + |\langle \bar{\Phi}_f(-\frac{1}{2}) | R_{10} | \bar{\Phi}_i(-\frac{1}{2}) \rangle|^2 + |\langle \bar{\Phi}_f(-\frac{3}{2}) | R_{11} | \bar{\Phi}_i(-\frac{1}{2}) \rangle|^2
 \end{aligned}
 \tag{1-13}$$

Carrying out the integration in eq.(1-13), the transition probability was found to be (3) (4)

$$T_E(1) = \begin{cases} 1.85 \times 10^{15} & \text{sec}^{-1} \\ 1.70 \times 10^{15} & \text{sec}^{-1} \end{cases}$$

The two values of $T_E(1)$ correspond to two different values of parameter β' in the wave functions. The level widths are then

$$\Gamma_r = \begin{cases} 1.23 & \text{ev} \\ 1.12 & \text{ev} \end{cases}$$

which is related to $T_E(1)$ by the equation

$$\Gamma_r = 0.66 \times 10^{-15} T_E(1) = \hbar T_E(1)$$

CHAPTER II

ALTERNATIVE FORMS OF THE ELECTRIC DIPOLE TRANSITION OPERATOR

In the previous chapter, it was shown how the operator R_{1m} can be used to calculate the electric dipole transition probability. R_{1m} depends only on the coordinates of the protons relative to the centre of mass of the nucleus. It will be shown in this chapter that an alternative form of this operator can be derived which depends on momentum, spin and coordinates of the particles.

1. Derivation of Operator ⁽⁹⁾

Let H denote the operator corresponding to the Hamiltonian of a nuclear system consisting of neutrons and protons.

$$H = \sum_{i=1}^A \frac{p_i^2}{2m} + V \quad (2-1)$$

where A is the mass number of the nucleus, and the potential energy V is in general a function of the coordinates, momenta and spins of all nucleons.

If $|f\rangle$ and $|i\rangle$ are two eigenstates of the hamiltonian H with energy eigenvalues E_f and E_i , then

$$H |f\rangle = E_f |f\rangle \quad (2-2)$$

$$H |i\rangle = E_i |i\rangle$$

Let

$$\vec{R}_p = \sum_i^Z \vec{r}_i \quad (2-3)$$

where \sum_i^Z denotes the summation of index i over all protons, and \vec{r}_i is the coordinate of particle i in the centre of mass system, i.e.

$$\vec{r}_i = \vec{r}_i - \vec{R}_{cm} \quad (2-4)$$

\vec{R}_{cm} being the position vector of the centre of mass.

Since there are two protons in the nucleus, by eqs.(2-3) and (2-4), we have

$$\vec{R}_p = \sum_i \vec{r}_i - 2 \vec{R}_{cm} = \vec{R}_p - 2 \vec{R}_{cm} .$$

The matrix element of the commutator of \vec{R}_p and H between $|f\rangle$ and $|i\rangle$ is then, by eq.(2-2)

$$\begin{aligned} \langle f | [\vec{R}_p, H] | i \rangle &= \langle f | \vec{R}_p H - H \vec{R}_p | i \rangle \\ &= (E_i - E_f) \langle f | \vec{R}_p | i \rangle \end{aligned} \quad (2-5)$$

From this equation, it is seen that the operator \vec{R}_p , whose components are linear combinations of R_{1m} , can be replaced by $[\vec{R}_p, H] / (E_i - E_f)$.

The commutation rule for x and p_x of any particle is

$$x p_x - p_x x = i \hbar$$

Multiplying both sides by p_x , we have

$$x p_x^2 - p_x x p_x = i \hbar p_x$$

$$\text{or } x p_x^2 - p_x (i \hbar + p_x x) = i \hbar p_x$$

$$x p_x^2 - p_x^2 x = 2 i \hbar p_x .$$

Adding the other two components, we obtain

$$\vec{r} p^2 - p^2 \vec{r} = 2 i \hbar \vec{p} \quad (2-6)$$

For \vec{r} and \vec{p} belonging to different particles,

$$\vec{r}_i p_j^2 - p_j^2 \vec{r}_i = 0 \quad (i \neq j) \quad (2-7)$$

Then

$$\begin{aligned} [\vec{R}_p, H] &= [\vec{R}_p - 2 \vec{R}_{cm}, H] \\ &= [\vec{R}_p, H] - 2 [\vec{R}_{cm}, H] \end{aligned}$$

$$= \left[\sum_j^Z \vec{r}_j, \frac{1}{2m} \sum_{i=1}^A p_i^2 + V \right] - \frac{2}{5} \left[\sum_{j=1}^A \vec{r}_j, \frac{1}{2m} \sum_{i=1}^A p_i^2 + V \right]$$

By eqs.(2-6) and (2-7), we have

$$\begin{aligned} & \left[\vec{R}_p, \Pi \right] \\ &= \frac{i\hbar}{m} \sum_j^Z \vec{p}_j + [\vec{R}_p, V] - \frac{2i\hbar}{5m} \sum_{i=1}^A \vec{p}_i - \frac{2}{5} \left[\sum_{i=1}^A \vec{r}_i, V \right] \\ &= \frac{i\hbar}{m} \left(\sum_j^Z \vec{p}_j - \frac{2}{5} \sum_{i=1}^A \vec{p}_i \right) + [\vec{R}_p, V] - \frac{2}{5} [\vec{R}', V] \end{aligned} \quad (2-8)$$

where

$$\vec{R}' = \sum_{i=1}^A \vec{r}_i = 5 \vec{R}_{cm} \quad (2-9)$$

2. Evaluation of $[\vec{R}_p, V]$ and $[\vec{R}', V]$

The explicit expression for V was chosen to be the Serber potential in the calculation of the energy levels of He^5 (2).

$$\begin{aligned} V_{ij} = & -V_0 \exp(-k r_{ij}^2) \left[w(1 + P_{ij}^s) + b(P_{ij}^\sigma - P_{ij}^\tau) \right] \\ & -V_{Ls} \exp(-\lambda r_{ij}^2) (\vec{r}_i - \vec{r}_j) \times (\vec{p}_i - \vec{p}_j) \cdot (\vec{\sigma}_i + \vec{\sigma}_j) \frac{1}{2\hbar} \end{aligned} \quad (2-10)$$

where $V_0 = 68.6$ Mev, $k = 4.16 \times 10^{25} \text{ cm}^{-2}$, $w = 0.41$, $b = 0.09$

and P_{ij}^s , P_{ij}^σ , P_{ij}^τ represent the space, spin and isotopic exchange operators respectively. $\vec{\sigma}_i$ is the Pauli spin operator. The range λ and depth V_{Ls} of the spin-orbit potential are also constants and will be discussed later.

The total potential energy is then

$$V = \sum_{\text{all pairs}} V_{ij}$$

Since r_i commutes with all coordinate and exchange operators, the commutator of \vec{R}_p and the first term in (2-10) vanishes, and only the term involving the spin-orbit potential remains.

Therefore, we have

$$[\vec{R}_p, V] = -\frac{V_{LS}}{2\hbar} \left[\sum_i \vec{r}_i, \sum'_{j,k} \exp(-\lambda r_{jk}^2) (\vec{r}_j - \vec{r}_k) \right. \\ \left. \times (\vec{p}_j - \vec{p}_k) \cdot (\vec{\sigma}_j + \vec{\sigma}_k) \right]$$

where j and k are summed over all pairs of nucleons, and

$\sum'_{j,k}$ denotes the summation excludes $j = k$. Then

$$[\vec{R}_p, V] = -\frac{V_{LS}}{2\hbar} \sum_i \sum'_{j,k} \left[\vec{r}_i, v_{jk} (\vec{r}_j - \vec{r}_k) \times (\vec{p}_j - \vec{p}_k) \cdot (\vec{\sigma}_j + \vec{\sigma}_k) \right] \\ = -\frac{V_{LS}}{2\hbar} \sum_i \sum'_{j,k} \left[\vec{r}_i, v_{jk} (\vec{r}_j \times \vec{p}_j + \vec{r}_k \times \vec{p}_k - \vec{r}_j \times \vec{p}_k - \vec{r}_k \times \vec{p}_j) \cdot (\vec{\sigma}_j + \vec{\sigma}_k) \right] \\ = -\frac{V_{LS}}{2\hbar} \sum_i \sum'_{j,k} v_{jk} \left\{ [\vec{r}_i, \vec{r}_j \times \vec{p}_j \cdot \vec{\sigma}_{jk}] + [\vec{r}_i, \vec{r}_k \times \vec{p}_k \cdot \vec{\sigma}_{jk}] \right. \\ \left. - [\vec{r}_i, \vec{r}_j \times \vec{p}_k \cdot \vec{\sigma}_{jk}] - [\vec{r}_i, \vec{r}_k \times \vec{p}_j \cdot \vec{\sigma}_{jk}] \right\} \quad (2-11)$$

where the following abbreviations have been used

$$v_{ij} = \exp(-\lambda r_{ij}^2)$$

$$\text{and } \vec{\sigma}_{ij} = \vec{\sigma}_i + \vec{\sigma}_j$$

Expanding the first bracket in eq.(2-11) into components yields

$$[\vec{r}_i, \vec{r}_j \times \vec{p}_j \cdot \vec{\sigma}_{jk}] \\ = \left[\vec{i} x_i + \vec{j} y_i + \vec{k} z_i, y_j p_{zj} \sigma_{xjk} - z_j p_{yj} \sigma_{xjk} + z_j p_{xj} \sigma_{yjk} \right. \\ \left. - x_j p_{zj} \sigma_{yjk} + x_j p_{yj} \sigma_{zjk} - y_j p_{xj} \sigma_{zjk} \right]$$

Using the fact that x_i commutes with \vec{r}_j , \vec{p}_j (any j) and \vec{p}_j ($j \neq i$), the x component reduces to

$$\begin{aligned} & [x_i, z_j p_{xj} \delta_{yjk} - y_j p_{xj} \delta_{zjk}] \\ &= [x_i, p_{xj}] z_j \delta_{yjk} - [x_i, p_{xj}] y_j \delta_{zjk} \\ &= i\hbar \delta_{ij} (z_j \delta_{yjk} - y_j \delta_{zjk}) \\ &= i\hbar (\vec{p}_{jk} \times \vec{r}_j)_x \delta_{ij} \end{aligned}$$

Similarly, the y and z components can be written as

$$[y_i, -z_j p_{yj} \delta_{xjk} + x_j p_{yj} \delta_{zjk}] = i\hbar (\vec{p}_{jk} \times \vec{r}_j)_y \delta_{ij}$$

$$\text{and } [z_i, y_j p_{zj} \delta_{xjk} - x_j p_{zj} \delta_{yjk}] = i\hbar (\vec{p}_{jk} \times \vec{r}_j)_z \delta_{ij}$$

$$\text{so } [\vec{r}_i, \vec{r}_j \times \vec{p}_j \cdot \vec{p}_{jk}] = i\hbar \vec{p}_{jk} \times \vec{r}_j \delta_{ij} \quad (2-12)$$

and by exchanging the subscripts j and k ,

$$[\vec{r}_i, \vec{r}_k \times \vec{p}_k \cdot \vec{p}_{jk}] = i\hbar \vec{p}_{jk} \times \vec{r}_k \delta_{ik} \quad (2-13)$$

Next, we shall calculate the third bracket in eq.(2-11), i.e. $[\vec{r}_i, \vec{r}_j \times \vec{p}_k \cdot \vec{p}_{jk}]$. By the same technique used above, the x component is

$$\begin{aligned} & [x_i, y_j p_{zk} \delta_{xjk} - z_j p_{yk} \delta_{xjk} + z_j p_{xk} \delta_{yjk} - x_j p_{zk} \delta_{yjk}] \\ &= [x_i, z_j p_{xk} \delta_{yjk} - y_j p_{xk} \delta_{zjk}] \\ &= i\hbar \delta_{ik} (z_j \delta_{yjk} - y_j \delta_{zjk}) \\ &= i\hbar (\vec{p}_{jk} \times \vec{r}_j)_x \delta_{ik} \end{aligned}$$

and the y and z components are

$$i\hbar (\vec{\sigma}_{jk} \times \vec{r}_j)_y \delta_{ik}$$

and $i\hbar (\vec{\sigma}_{jk} \times \vec{r}_j)_z \delta_{ik}$

respectively.

Hence,

$$[\vec{r}_i, \vec{r}_j \times \vec{p}_k \cdot \vec{\sigma}_{jk}] = i\hbar (\vec{\sigma}_{jk} \times \vec{r}_j) \delta_{ik} \quad (2-14)$$

and $[\vec{r}_i, \vec{r}_k \times \vec{p}_j \cdot \vec{\sigma}_{jk}] = i\hbar (\vec{\sigma}_{jk} \times \vec{r}_k) \delta_{ij} \quad (2-15)$

From eq.(2-12) to eq.(2-15), we have

$$\begin{aligned} [\vec{R}_p, V] &= -\frac{iV_{LS}}{2} \sum_i \sum'_{j,k} v_{jk} (\vec{\sigma}_{jk} \times \vec{r}_j \delta_{ij} + \vec{\sigma}_{jk} \times \vec{r}_k \delta_{ik} \\ &\quad - \vec{\sigma}_{jk} \times \vec{r}_j \delta_{ik} - \vec{\sigma}_{jk} \times \vec{r}_k \delta_{ij}) \\ &= -iV_{LS} \sum_i \sum'_{jk} v_{jk} \vec{\sigma}_{jk} \times \vec{r}_j (\delta_{ij} - \delta_{ik}) \end{aligned} \quad (2-16)$$

The last step arises simply from an exchange of the dummy indices j and k.

Summing over j and k first, and making use of the property of the Kronecker delta δ_{ij} , eq.(2-16) becomes

$$\begin{aligned} [\vec{R}_p, V] &= -\frac{iV_{LS}}{2} \sum_i \left(\sum_{k=1}^A v_{ik} \vec{\sigma}_{ik} \times \vec{r}_i - \sum_{j=1}^A v_{ji} \vec{\sigma}_{ji} \times \vec{r}_j \right) \\ &= -\frac{iV_{LS}}{2} \sum_i \sum_{j=1}^A v_{ij} \vec{\sigma}_{ij} \times (\vec{r}_i - \vec{r}_j) \end{aligned} \quad (2-17)$$

The factor $\frac{1}{2}$ arises because j and k are summed only over pairs

of particles. The condition $j \neq k$ is taken into account automatically because of the appearance of $\delta_{ij} - \delta_{ik}$.

Eq.(2-17) vanishes if the index i is summed over all nucleons. By eq.(2-9), $[\vec{R}', V]$ differs from $[\vec{R}_p, V]$ only in the summation over index i . We have therefore

$$[\vec{R}', V] = 0$$

The purpose of calculating $[\vec{R}_p, V]$ was to allow the evaluation of $[\vec{R}_p, H]$, in order to use explicitly the relation

$$\begin{aligned} \vec{R}_p &\rightarrow \frac{1}{E_i - E_f} [\vec{R}_p, H] \\ &= \frac{2\pi}{\hbar c k} \frac{i\hbar}{m} \left(\sum_i \vec{p}_i - \frac{2}{5} \sum_{i=1}^A \vec{p}_i \right) - \frac{iV_{LS}}{2} \sum_i \sum_{j=1}^A v_{ij} \vec{\sigma}_{ij} \times (\vec{r}_i - \vec{r}_j) \\ &\equiv \vec{K} + \vec{V} \end{aligned} \quad (2-18)$$

where k is the wave number defined by

$$k = \frac{2\pi}{\lambda} \quad (2-19)$$

and λ is the wave length related to the energy difference by

$$E_i - E_f = \frac{\hbar c}{\lambda} \quad (2-20)$$

The operator R_{1m} in eq.(1-13) can now be written in terms of the Cartesian components of \vec{R}_p .

$$R_{1m} = \sum_i \bar{r}_i Y_1^{m*}(\omega_i) \quad (2-21)$$

$$\begin{aligned} R_{10} &= \sum_i \bar{r}_i Y_1^{0*}(\omega_i) \\ &= \sqrt{\frac{3}{4\pi}} \sum_i \bar{z}_i = \sqrt{\frac{3}{4\pi}} \bar{R}_z \end{aligned} \quad (2-22)$$

$$\begin{aligned}
 R_{1\pm 1} &= \sum_i \bar{r}_i Y_1^{\pm 1*}(\omega_i) = (\pm 1) \left(-\sqrt{\frac{3}{8\pi}}\right) \sum_i \bar{r}_i e^{\mp i\phi_i} \sin \theta_i \\
 &= \mp \sqrt{\frac{3}{8\pi}} \sum_i (\bar{x}_i \mp i \bar{y}_i) \\
 &= \mp \sqrt{\frac{3}{8\pi}} (\bar{R}_x \mp i \bar{R}_y) \qquad (2-23)
 \end{aligned}$$

Therefore, the transition probability can be calculated by using the components of the right hand side of eq.(2-18), where the momentum operator \vec{p} is replaced by $-i\hbar\vec{\nabla}$.

With the initial and final state wave functions explicitly known, and all constants in the potential given, the calculation is straightforward but tedious and lengthy. The details are given in the next chapter.

CHAPTER III

MATRIX ELEMENT OF THE MOMENTUM OPERATOR

In the previous chapter, it was shown that the coordinate operator can be replaced by the sum of a momentum operator and an operator proportional to the spin-orbit potential. The evaluation of the former will be done in detail in this chapter.

From eq.(1-13), the square of the matrix element is

$$\begin{aligned}
 B_E(1) &= \sum_{M_i, M_f} |\langle f | R_{1m} | i \rangle|^2 \\
 &= \sum_{M_i, M_f} |\langle f | K_{1m} + V_{1m} | i \rangle|^2 \\
 &= \sum_{M_i, M_f} |\langle f | K_{1m} | i \rangle + \langle f | V_{1m} | i \rangle|^2 \quad (3-1)
 \end{aligned}$$

where K_{1m} and V_{1m} are related to \vec{K} and \vec{V} in the same manner as R_{1m} is related to \vec{R}_p in eqs.(2-22) and (2-23).

When a scalar product of two wave functions $\langle \psi_1 | \psi_2 \rangle$ is to be computed, the spin coordinates are summed up first. The remaining terms are products whose spin coordinates are the same in both states; this follows from the orthogonality property of the spin wave functions. Therefore, when we make the replacement of \vec{R}_p by $\frac{\hbar}{mck} \vec{V}$, the spatial wave functions on both sides of the operator are the same as those used by Tran Duc⁽³⁾, because neither \vec{R}_p nor $\frac{\hbar}{mck} \vec{V}$ contain spin operators.

The matrix elements $\langle f | R_{1m} | i \rangle$ in eq.(1-13), after the summations over spin coordinates are carried out, are found to be⁽³⁾

$$\langle \bar{\Phi}_f(\frac{3}{2}) | R_{1-1} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{6 \sqrt{2}} \langle (5234;1)_{1-} (1234;5)_1 | R_{1-1} | (123;45) \rangle \quad (3-2)$$

$$\langle \bar{\Phi}_f(\frac{1}{2}) | R_{10} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{6 \sqrt{3}} \langle (5234;1)_0 (1234;5)_0 | R_{10} | (123;45) \rangle \quad (3-3)$$

$$\langle \bar{\Phi}_f(\frac{1}{2}) | R_{1-1} | \varphi_i(-\frac{1}{2}) \rangle = \frac{N_i N_f}{6 \sqrt{6}} \langle (5234;1)_{1-} (1234;5)_1 | R_{1-1} | (123;45) \rangle \quad (3-4)$$

$$\langle \bar{\Phi}_f(-\frac{1}{2}) | R_{11} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{6 \sqrt{6}} \langle (5234;1)_{-1} (1234;5)_{-1} | R_{11} | (123;45) \rangle \quad (3-5)$$

$$\langle \bar{\Phi}_f(-\frac{1}{2}) | R_{10} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{6 \sqrt{3}} \langle (5234;1)_0 (1234;5)_0 | R_{10} | (123;45) \rangle \quad (3-6)$$

$$\langle \bar{\Phi}_f(-\frac{3}{2}) | R_{11} | \varphi_i(-\frac{1}{2}) \rangle = \frac{N_i N_f}{6 \sqrt{2}} \langle (5234;1)_{-1} (1234;5)_{-1} | R_{11} | (123;45) \rangle \quad (3-7)$$

To calculate the matrix element of K_{1m} , we only need to replace R_{1m} by a differential operator according to eqs.(2-18), (2-22) and (2-23). For example, R_{10} is replaced by

$$\begin{aligned} & \frac{i}{\hbar c k} \frac{i \hbar}{m} \frac{\hbar}{i \sqrt{4 \pi}} \left(\sum_i \frac{\partial}{\partial z_i} - \frac{2}{5} \sum_{i=1}^A \frac{\partial}{\partial z_i} \right) \\ &= \frac{\hbar}{m c k} \sqrt{\frac{3}{4 \pi}} \left(\sum_i \frac{\partial}{\partial z_i} - \frac{2}{5} \sum_{i=1}^A \frac{\partial}{\partial z_i} \right) \end{aligned} \quad (3-8)$$

Let

$$I_m = \langle (5234;1)_m (1234;5)_m | K_{1-m} | (123;45) \rangle \quad (3-9)$$

with $m = 0, \pm 1$. Also let

$$D_{0i} = \sqrt{\frac{3}{4 \pi}} \frac{\partial}{\partial z_i} \quad (3-10)$$

$$D_{\pm 1i} = \mp \sqrt{\frac{3}{8 \pi}} \left(\frac{\partial}{\partial x_i} \mp i \frac{\partial}{\partial y_i} \right) \quad (3-11)$$

Then, analogous to eq.(3-8), K_{1m} becomes

$$K_{1-m} = \frac{\hbar}{mck} \left(\sum_i^Z D_{-mi} - \frac{2}{5} \sum_{i=1}^A D_{-mi} \right) \quad (3-12)$$

and eq.(3-9) can be written as

$$\begin{aligned} I_m &= \frac{\hbar}{mck} \langle (5234;1)_m - (1234;5)_m \left| \sum_i^Z D_{-mi} - \frac{2}{5} \sum_{i=1}^A D_{-mi} \right| (123;45) \rangle \\ &= \frac{\hbar}{mck} (L_{1m} - L_{2m}) \end{aligned} \quad (3-13)$$

where

$$L_{1m} = \langle (5234;1)_m \left| \sum_i^Z D_{-mi} - \frac{2}{5} \sum_{i=1}^A D_{-mi} \right| (123;45) \rangle \quad (3-14)$$

$$L_{2m} = \langle (1234;5)_m \left| \sum_i^Z D_{-mi} - \frac{2}{5} \sum_{i=1}^A D_{-mi} \right| (123;45) \rangle \quad (3-15)$$

1. Evaluation of L_{1m}

The explicit form of $(5234;1)_m^*$ is given by eq.(1-3), i.e.

$$(5234;1)_m^* = \exp\left(-\frac{\alpha_1}{2} \sum_i r_i'^2\right) R_1 Y_1^{m*}(\Omega_1) e^{-\frac{2\beta'}{5} R_1^2} e^{-\frac{5r}{2} R_{cm}^2} \quad (3-16)$$

where

$$\begin{aligned} \vec{r}_i'' &= \vec{r}_i - \vec{R}_\alpha \quad (i = 5, 2, 3, 4) \\ \vec{R}_\alpha &= \frac{1}{4} (\vec{r}_5 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) \\ \vec{R}_1 &= \vec{R}_\alpha - \vec{r}_1 \\ \vec{R}_{cm} &= \frac{1}{5} (\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4 + \vec{r}_5) \end{aligned} \quad (3-17)$$

For convenience of calculation, we first transform the wave function to the system with $\vec{R}, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{R}_{cm}$ as new

coordinates. The transformation equations are

$$\begin{aligned}
 \vec{r}_1 &= \frac{6}{5} \vec{R} - \vec{r}_2 - \vec{r}_3 + \vec{R}_{cm} \\
 \vec{r}_2 &= \vec{r}_2 + \vec{R}_{cm} \\
 \vec{r}_3 &= \vec{r}_3 + \vec{R}_{cm} \\
 \vec{r}_4 &= \vec{r}_4 + \vec{R}_{cm} \\
 \vec{r}_5 &= -\frac{6}{5} \vec{R} - \vec{r}_4 + \vec{R}_{cm}
 \end{aligned} \tag{3-18}$$

where \vec{R} is the relative coordinate of the deuteron and the triton in (123;45). It is seen that eq.(3-18) is consistent with the definition of \vec{R} in eq.(1-8). The reasons for choosing this particular transformation with \vec{R} and \vec{R}_{cm} as new coordinates are that the factor R^2 appears in (123;45) and the motion of the centre of mass can be separated from the other variables, as can be seen later. This will simplify the calculation.

The Jacobian of the transformation is

$$J_1 = \frac{\partial (\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{r}_5)}{\partial (\vec{R}, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{R}_{cm})} = 6 .$$

Using eq.(3-18), the quantities in eq.(3-16) can be expressed in terms of the new coordinates as follow:

$$\begin{aligned}
 r_2'^2 &= \frac{1}{16} \left(\frac{36}{25} R^2 + 9 \vec{r}_2^2 + \vec{r}_3^2 + \frac{36}{5} \vec{R} \cdot \vec{r}_2 - \frac{12}{5} \vec{R} \cdot \vec{r}_3 - 6 \vec{r}_2 \cdot \vec{r}_3 \right) \\
 r_3'^2 &= \frac{1}{16} \left(\frac{36}{25} R^2 + \vec{r}_2^2 + 9 \vec{r}_3^2 - \frac{12}{5} \vec{R} \cdot \vec{r}_2 + \frac{36}{5} \vec{R} \cdot \vec{r}_3 - 6 \vec{r}_2 \cdot \vec{r}_3 \right)
 \end{aligned}$$

$$r_4'^2 = \frac{1}{16} \left(\frac{36}{25} R^2 + \bar{r}_2^2 + \bar{r}_3^2 + 16 \bar{r}_4^2 - \frac{12}{5} \bar{R} \cdot \bar{r}_2 - \frac{12}{5} \bar{R} \cdot \bar{r}_3 \right. \\ \left. + 2 \bar{r}_2 \cdot \bar{r}_3 - 8 \bar{r}_2 \cdot \bar{r}_4 - 8 \bar{r}_3 \cdot \bar{r}_4 \right)$$

$$r_5'^2 = \frac{1}{16} \left(\frac{18^2}{25} R^2 + \bar{r}_2^2 + \bar{r}_3^2 + 16 \bar{r}_4^2 + \frac{36}{5} \bar{R} \cdot \bar{r}_2 + \frac{36}{5} \bar{R} \cdot \bar{r}_3 \right. \\ \left. + \frac{144}{5} \bar{R} \cdot \bar{r}_4 + 2 \bar{r}_2 \cdot \bar{r}_3 + 8 \bar{r}_2 \cdot \bar{r}_4 + 8 \bar{r}_3 \cdot \bar{r}_4 \right)$$

$$R_1^2 = \frac{1}{16} \left(36 R^2 + 25 \bar{r}_2^2 + 25 \bar{r}_3^2 - 60 \bar{R} \cdot \bar{r}_2 - 60 \bar{R} \cdot \bar{r}_3 + 50 \bar{r}_2 \cdot \bar{r}_3 \right)$$

$$R_1 Y_1^{m*}(\Omega_1) = \frac{1}{4} \left(-6 R Y_1^{m*}(\Omega) + 5 \bar{r}_2 Y_1^{m*}(\omega_2) + 5 \bar{r}_3 Y_1^{m*}(\omega_3) \right)$$

where $R, \bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4$ are the magnitudes of $\vec{R}, \vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4$.

Eq.(3-16) can then be written as

$$(5234;1)_m^* = \frac{1}{4} \left[-6 R Y_1^{m*}(\Omega) + 5 \bar{r}_2 Y_1^{m*}(\omega_2) + 5 \bar{r}_3 Y_1^{m*}(\omega_3) \right] \\ \cdot \exp \left[- \left(A_1 R^2 + B_1 \bar{r}_2^2 + C_1 \bar{r}_3^2 + D_1 \bar{r}_4^2 + E_1 R_{cm}^2 + F_1 \bar{R} \cdot \bar{r}_2 \right. \right. \\ \left. \left. + G_1 \bar{R} \cdot \bar{r}_3 + H_1 \bar{R} \cdot \bar{r}_4 + I_1 \bar{r}_2 \cdot \bar{r}_3 + J_1 \bar{r}_2 \cdot \bar{r}_4 + K_1 \bar{r}_3 \cdot \bar{r}_4 \right) \right] \quad (3-19)$$

The exponential will be abbreviated to $\exp(-\phi_1)$.

The coefficients A_1, B_1, \dots, K_1 are functions of the variational parameters. Their forms and numerical values are given in Appendix B.

It is interesting to note here that the transformed wave function contains \bar{R}_{cm} only in the exponential. It will be seen later that the same situation occurs in (123;45).

In fact, in the matrix element, the only dependence on R_{cm} is of the form

$$\int \psi_{cm}^* \psi_{cm} d^3 R_{cm} = 1,$$

and so in calculating L_{lm} , the integration over \vec{R}_{cm} can be separated from the other variables and will be dropped.

The ~~final~~ ^{initial} state wave function (123;45) can also be transformed by eq.(3-18) to the new coordinate system. It is

$$(123;45) = \exp \left(-\frac{\alpha}{2} \sum_{i=1}^3 r_i'^2 - \frac{\alpha}{2} \sum_{j=4}^5 r_j'^2 \right) R^2 \cdot e^{-\frac{3\beta}{5} R^2} \cdot e^{-\frac{5r}{2} R_{cm}^2} \quad (3-20)$$

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

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

$$\vec{R}_t = \frac{1}{3} (\vec{r}_1 + \vec{r}_2 + \vec{r}_3) \quad (3-21)$$

$$\vec{R}_d = \frac{1}{2} (\vec{r}_4 + \vec{r}_5)$$

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

By eq.(3-18), this becomes

$$\begin{aligned} (123;45) &= R^2 \exp \left[- (A_2 R^2 + B_2 \vec{r}_2^2 + C_2 \vec{r}_3^2 + D_2 \vec{r}_4^2 + E_2 R_{cm}^2 \right. \\ &\quad \left. + F_2 \vec{R} \cdot \vec{r}_2 + G_2 \vec{R} \cdot \vec{r}_3 + H_2 \vec{R} \cdot \vec{r}_4 + I_2 \vec{r}_2 \cdot \vec{r}_3 + J_2 \vec{r}_2 \cdot \vec{r}_4 + K_2 \vec{r}_3 \cdot \vec{r}_4) \right] \\ &= R^2 \exp (-\phi_2) \quad (3-22) \end{aligned}$$

The numerical values of the coefficients A_2, B_2, \dots, K_2 and their dependence on the variational parameters are given in Appendix B.

It is now clear that the particular choice of the transformation, eq.(3-18), is most appropriate for this problem because \bar{R} is an independent variable, and hence R^2 in (123;45) need not be transformed into a quadratic form.

The operators in eq.(3-14) must now be expressed in terms of the new coordinate system.

$$\frac{\partial}{\partial z_3} = \frac{\partial Z}{\partial z_3} \frac{\partial}{\partial Z} + \frac{\partial \bar{z}_2}{\partial z_3} \frac{\partial}{\partial \bar{z}_2} + \frac{\partial \bar{z}_3}{\partial z_3} \frac{\partial}{\partial \bar{z}_3} + \frac{\partial \bar{z}_4}{\partial z_3} \frac{\partial}{\partial \bar{z}_4} + \frac{\partial Z_{cm}}{\partial z_3} \frac{\partial}{\partial Z_{cm}}$$

Using the transformation inverse to eq.(3-18), i.e.

$$\bar{R} = \frac{1}{3} \bar{r}_1 + \frac{1}{3} \bar{r}_2 + \frac{1}{3} \bar{r}_3 - \frac{1}{2} \bar{r}_5$$

$$\bar{r}_2 = -\frac{1}{5} \bar{r}_1 + \frac{4}{5} \bar{r}_2 - \frac{1}{5} \bar{r}_3 - \frac{1}{5} \bar{r}_4 - \frac{1}{5} \bar{r}_5$$

$$\bar{r}_3 = -\frac{1}{5} \bar{r}_1 - \frac{1}{5} \bar{r}_2 + \frac{4}{5} \bar{r}_3 - \frac{1}{5} \bar{r}_4 - \frac{1}{5} \bar{r}_5$$

$$\bar{r}_4 = -\frac{1}{5} \bar{r}_1 - \frac{1}{5} \bar{r}_2 - \frac{1}{5} \bar{r}_3 + \frac{4}{5} \bar{r}_4 - \frac{1}{5} \bar{r}_5$$

$$\bar{R}_{cm} = \frac{1}{5} (\bar{r}_1 + \bar{r}_2 + \bar{r}_3 + \bar{r}_4 + \bar{r}_5) ,$$

this becomes

$$\frac{\partial}{\partial z_3} = \frac{1}{3} \frac{\partial}{\partial Z} - \frac{1}{5} \frac{\partial}{\partial \bar{z}_2} + \frac{4}{5} \frac{\partial}{\partial \bar{z}_3} - \frac{1}{5} \frac{\partial}{\partial \bar{z}_4} + \frac{1}{5} \frac{\partial}{\partial Z_{cm}}$$

Similarly,

$$\frac{\partial}{\partial z_4} = -\frac{1}{2} \frac{\partial}{\partial Z} - \frac{1}{5} \frac{\partial}{\partial z_2} - \frac{1}{5} \frac{\partial}{\partial z_3} + \frac{4}{5} \frac{\partial}{\partial z_4} + \frac{1}{5} \frac{\partial}{\partial Z_{cm}}$$

and
$$\sum_{i=1}^5 \frac{\partial}{\partial z_i} = \frac{\partial}{\partial Z_{cm}}$$

and so

$$\sum_{i=3}^4 \frac{\partial}{\partial z_i} - \frac{2}{5} \sum_{i=1}^5 \frac{\partial}{\partial z_i} = -\frac{1}{6} \frac{\partial}{\partial Z} - \frac{2}{5} \frac{\partial}{\partial z_2} + \frac{3}{5} \frac{\partial}{\partial z_3} + \frac{3}{5} \frac{\partial}{\partial z_4}$$

(3-23)

Similar equations can be written for the x and y components.

Let

$$D'_{-m} = \sum_{i=3}^4 D_{-mi} - \frac{2}{5} \sum_{i=1}^5 D_{-mi} ; \quad (3-24)$$

by eqs.(3-10) and (3-11),

$$\begin{aligned} D'_0 &= \sqrt{\frac{3}{4\pi}} \left(-\frac{1}{6} \frac{\partial}{\partial Z} - \frac{2}{5} \frac{\partial}{\partial z_2} + \frac{3}{5} \frac{\partial}{\partial z_3} + \frac{3}{5} \frac{\partial}{\partial z_4} \right) \\ D'_{\pm 1} &= \mp \sqrt{\frac{3}{8\pi}} \left[-\frac{1}{6} \left(\frac{\partial}{\partial X} \mp i \frac{\partial}{\partial Y} \right) - \frac{2}{5} \left(\frac{\partial}{\partial x_2} \mp i \frac{\partial}{\partial y_2} \right) \right. \\ &\quad \left. + \frac{3}{5} \left(\frac{\partial}{\partial x_3} \mp i \frac{\partial}{\partial y_3} \right) + \frac{3}{5} \left(\frac{\partial}{\partial x_4} \mp i \frac{\partial}{\partial y_4} \right) \right] \end{aligned} \quad (3-25)$$

Combining eqs.(3-14), (3-19), (3-22) and (3-24), L_{1m} can be written as

$$\begin{aligned} L_{1m} &= \langle (5234; 1)_m | D'_{-m} | (123; 45) \rangle \\ &= \frac{|J_1|^3}{4} \int \left[-6 R Y_1^{m*}(\Omega) + 5 \bar{r}_2 Y_1^{m*}(\omega_2) + 5 \bar{r}_3 Y_1^{m*}(\omega_3) \right] \\ &\quad D'_{-m} \left[R^2 \exp(-\phi_2) \right] d\tau \end{aligned} \quad (3-26)$$

where $d\tau = d^3R d^3\bar{r}_2 d^3\bar{r}_3 d^3\bar{r}_4 d^3R_{cm}$

Now

$$\begin{aligned}
 & D'_0 \left[R^2 \exp (-\phi_2) \right] \\
 &= (D'_0 R^2 - R^2 D'_0 \phi_2) \exp (-\phi_2) \\
 &= \sqrt{\frac{3}{4\pi}} \left[-\frac{1}{3} Z - R^2 \left(-\frac{1}{3} A_2 - \frac{2}{5} F_2 + \frac{3}{5} G_2 + \frac{3}{5} H_2 \right) Z \right. \\
 &\quad + \left(-\frac{1}{6} F_2 - \frac{4}{5} B_2 + \frac{3}{5} I_2 + \frac{3}{5} J_2 \right) \bar{z}_2 + \left(-\frac{1}{6} G_2 - \frac{2}{5} C_2 \right. \\
 &\quad \left. \left. + \frac{3}{5} K_2 \right) \bar{z}_3 + \left(-\frac{1}{6} H_2 - \frac{2}{5} J_2 + \frac{3}{5} K_2 + \frac{6}{5} D_2 \right) \bar{z}_4 \right] \exp (-\phi_2) \\
 &= \sqrt{\frac{3}{4\pi}} \left[-\frac{1}{3} Z - R^2 (f_1 Z + f_2 \bar{z}_2 + f_3 \bar{z}_3 + f_4 \bar{z}_4) \right] \exp (-\phi_2) \\
 &= \left\{ -\frac{1}{3} R Y_1^0(\Omega) - R^2 [f_1 R Y_1^0(\Omega) + f_2 \bar{r}_2 Y_1^0(\omega_2) + f_3 \bar{r}_3 Y_1^0(\omega_3) \right. \\
 &\quad \left. + f_4 \bar{r}_4 Y_1^0(\omega_4) \right\} \exp (-\phi_2) \quad (3-27)
 \end{aligned}$$

where $f_1, f_2, f_3,$ and f_4 are defined by eq.(3-27).

Similarly, it can be shown that

$$\begin{aligned}
 & D'_{\pm 1} \left[R^2 \exp (-\phi_2) \right] \\
 &= - \left\{ -\frac{1}{3} R Y_1^{-1}(\Omega) - R^2 [f_1 R Y_1^{-1}(\Omega) + f_2 \bar{r}_2 Y_1^{-1}(\omega_2) + f_3 \bar{r}_3 Y_1^{-1}(\omega_3) \right. \\
 &\quad \left. + f_4 \bar{r}_4 Y_1^{-1}(\omega_4) \right\} \exp (-\phi_2) \quad (3-28)
 \end{aligned}$$

It is to be noted that only negative signs (instead of \bar{r}) appear and that the spherical harmonics have $m = -1$.

Eq.(3-26) then becomes

$$\begin{aligned}
 L_{1m} = & (-1)^m \frac{|J_1|^3}{4} \int \left\{ -6 R Y_1^{m*}(\Omega) + 5 \bar{r}_2 Y_1^{m*}(\omega_2) + 5 \bar{r}_3 Y_1^{m*}(\omega_3) \right\} \cdot \\
 & \left\{ -\frac{1}{3} R Y_1^m(\Omega) - [R^2 f_1 R Y_1^m(\Omega) + f_2 \bar{r}_2 Y_1^m(\omega_2) + f_3 \bar{r}_3 Y_1^m(\omega_3) \right. \\
 & \left. + f_4 \bar{r}_4 Y_1^m(\omega_4) \right\} \exp (-\phi) d\tau \quad (3-29)
 \end{aligned}$$

with $\phi = \phi_1 + \phi_2$

$$\begin{aligned}
 &= (A_1 + A_2) R^2 + (B_1 + B_2) \bar{r}_2^2 + \dots + (K_1 + K_2) \bar{r}_3 \cdot \bar{r}_4 \\
 &= AR^2 + B\bar{r}_2^2 + C\bar{r}_3^2 + D\bar{r}_4^2 + E R_{cm}^2 + F \bar{R} \cdot \bar{r}_2 + G \bar{R} \cdot \bar{r}_3 \\
 &\quad + H \bar{R} \cdot \bar{r}_4 + I \bar{r}_2 \cdot \bar{r}_3 + J \bar{r}_2 \cdot \bar{r}_4 + K \bar{r}_3 \cdot \bar{r}_4
 \end{aligned}$$

In order to evaluate the integral in eq.(3-29), it is necessary to eliminate the cross-product terms in ϕ . A further transformation of the coordinates will be used to accomplish this reduction.

These kinds of transformations are not unique. Since R^2 appears in eq.(3-29), it is most convenient to have one of the new variables equal (or proportional) to \bar{R} . The method of finding such a transformation is given in Appendix C.

Let $\bar{\rho}_1, \bar{\rho}_2, \bar{\rho}_3, \bar{\rho}_4$ and $\bar{\rho}_5$ be the new variables.

The transformation equations are

$$\begin{aligned}
 \bar{R} &= \bar{\rho}_1 \\
 \bar{r}_2 &= a_{21} \bar{\rho}_1 + \bar{\rho}_2 + a_{23} \bar{\rho}_3 + a_{24} \bar{\rho}_4 \\
 \bar{r}_3 &= a_{31} \bar{\rho}_1 + \bar{\rho}_3 + a_{34} \bar{\rho}_4 \\
 \bar{r}_4 &= a_{41} \bar{\rho}_1 + \bar{\rho}_4 \\
 \bar{R}_{cm} &= \bar{\rho}_5
 \end{aligned} \tag{3-30}$$

where the a's are constants related to A, B, C,, K as given in Appendix C.

The Jacobian of this transformation is

$$J_2 = \frac{\partial (\bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4, \bar{r}_5)}{\partial (\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3, \vec{\rho}_4, \vec{\rho}_5)} = 1$$

By eq.(3-30), L_{1m} can be expressed in terms of the new variables as

$$\begin{aligned} L_{1m} = & (-1)^m \frac{|J_1|^3 |J_2|^3}{4} \int \left[e_1 \rho_1 Y_1^{m*}(\Omega_1) + e_2 \rho_2 Y_2^{m*}(\Omega_2) \right. \\ & + e_3 \rho_3 Y_3^{m*}(\Omega_3) + e_4 \rho_4 Y_4^{m*}(\Omega_4) \left. \right] \left\{ -\frac{1}{3} \rho_1 Y_1^m(\Omega_1) \right. \\ & - \rho_1^2 [c_1 \rho_1 Y_1^m(\Omega_1) + c_2 \rho_2 Y_2^m(\Omega_2) + c_3 \rho_3 Y_3^m(\Omega_3) \\ & + c_4 \rho_4 Y_4^m(\Omega_4)] \left. \right\} \exp[-(A_0 \rho_1^2 + B \rho_2^2 + C_0 \rho_3^2 + D_0 \rho_4^2)] \\ & d\vec{\rho}_1 d\vec{\rho}_2 d\vec{\rho}_3 d\vec{\rho}_4 \int e^{-E\rho_5^2} d\vec{\rho}_5 \end{aligned} \quad (3-31)$$

where $\Omega_1, \Omega_2, \Omega_3, \Omega_4$ and Ω_5 are the solid angles of $\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3, \vec{\rho}_4$ and $\vec{\rho}_5$; and

$$e_1 = -6 + 5 a_{21} + 5 a_{31}$$

$$e_2 = 5$$

$$e_3 = 5 a_{23} + 5$$

$$e_4 = 5 a_{24} + 5 a_{34}$$

$$c_1 = f_1 + a_{21} f_2 + a_{31} f_3 + a_{41} f_4$$

$$c_2 = f_2$$

(3-32)

$$c_3 = a_{23}f_2 + f_3 \quad (3-33)$$

$$c_4 = a_{24}f_2 + a_{34}f_3 + f_4$$

$$C_0 = C - \frac{I^2}{4B}$$

$$D_0 = D - \frac{J^2}{2B} - \frac{(K - \frac{JI}{2B})^2}{4C_0} \quad (3-34)$$

$$A_0 = A - \frac{F^2}{4B} - \frac{(G - \frac{FI}{2B})^2}{4C_0} - \frac{1}{4D_0} \left[H - \frac{FJ}{2B} - \frac{1}{2C_0} (G - \frac{FI}{2B})(K - \frac{JI}{2B}) \right]^2$$

The numerical values of these constants are given in Appendix D.

From eq.(3-31), it is obvious that the motion of the centre of mass (\vec{p}_5) is separated from the relative motion of the clusters. The last integral involving \vec{p}_5 in eq.(3-31) can be dropped, since in calculating the normalization constants, this factor also appeared, and hence it can be cancelled.

The volume element can be separated into radial and angular parts.

$$\begin{aligned} d\vec{p}_1 &= \rho_1^2 \sin \theta_1 d\theta_1 d\varphi_1 d\rho_1 \\ &= \rho_1^2 d\rho_1 d\Omega_1 \end{aligned}$$

Similar expressions can be written for $d\vec{p}_2$, $d\vec{p}_3$, $d\vec{p}_4$. In eq.(3-31), it is seen that all variables are separable and the integral can be carried out analytically term by term.

Making use of the orthonormality properties of the spherical harmonics, i.e.

$$\int Y_1^{m*}(\Omega) Y_1^{m'}(\Omega) d\Omega = \delta_{11} \delta_{mm'} \quad (3-35)$$

it is found that the non-vanishing terms in eq.(3-31) are

$$\begin{aligned} L_{1m} = & (-1)^{m+1} \frac{|J_1|^3}{4} \int \left\{ \frac{1}{3} e_1 \rho_1^2 Y_1^{m*}(\Omega_1) Y_1^m(\Omega_1) \right. \\ & + \rho_1^2 [c_1 e_1 \rho_1^2 Y_1^{m*}(\Omega_1) Y_1^m(\Omega_1) + c_2 e_2 \rho_2^2 Y_1^{m*}(\Omega_2) Y_1^m(\Omega_2) \\ & + c_3 e_3 \rho_3^2 Y_1^{m*}(\Omega_3) Y_1^m(\Omega_3) + c_4 e_4 \rho_4^2 Y_1^{m*}(\Omega_4) Y_1^m(\Omega_4)] \left. \right\} \\ & \rho_1^2 \rho_2^2 \rho_3^2 \rho_4^2 \exp[-(A_0 \rho_1^2 + B \rho_2^2 + C_0 \rho_3^2 + D_0 \rho_4^2)] \\ & d\rho_1 d\rho_2 d\rho_3 d\rho_4 d\Omega_1 d\Omega_2 d\Omega_3 d\Omega_4 \quad (3-36) \end{aligned}$$

Using eq.(3-35) and carrying out the integration, we have

$$\begin{aligned} L_{1m} = & (-1)^{m+1} \frac{81}{4} \frac{\pi^5}{A_0(A_0 B C_0 D_0)} \left(\frac{e_1}{3} + \frac{5 e_1 c_1}{2 A_0} + \frac{3 e_2 c_2}{2 B} \right. \\ & \left. + \frac{3 e_3 c_3}{2 C_0} + \frac{3 e_4 c_4}{2 D_0} \right) \quad (3-37) \end{aligned}$$

2. Evaluation of L_{2m}

The evaluation of L_{2m} can be done in exactly the same way as that of L_{1m} .

$$(1234;5)_m^* = \exp\left(-\frac{\alpha_1}{2} \sum_{i=1}^4 r_i'^2\right) R_1 Y_1^{m*}(\Omega_1) e^{-\frac{2\beta}{5} R_1^2} e^{-\frac{5r}{2} R_{cm}^2} \quad (3-38)$$

with

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

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

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

By eq.(3-18), this wave function is transformed from the $\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{r}_5$ system to the $\vec{R}, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{R}_{cm}$ system.

$$\begin{aligned} (1234;5)_m^* = \frac{1}{4} [& 6 R Y_1^{m*}(\Omega) + 5 \vec{r}_4 Y_1^{m*}(\omega_4)] \exp [- (A'_1 R^2 \\ & + B' \vec{r}_2^2 + C' \vec{r}_3^2 + D' \vec{r}_4^2 + E' R_{cm}^2 + F' \vec{R} \cdot \vec{r}_2 \\ & + G' \vec{R} \cdot \vec{r}_3 + H' \vec{R} \cdot \vec{r}_4 + I' \vec{r}_2 \cdot \vec{r}_3 + J' \vec{r}_2 \cdot \vec{r}_4 \\ & + K' \vec{r}_3 \cdot \vec{r}_4)] \end{aligned} \quad (3-39)$$

The numerical values of A', B', C', \dots, K' are given in Appendix B.

$$L_{2m} = \langle (1234;5)_m | D_{-m3} + D_{-m4} - \frac{2}{5} \sum_{i=1}^5 D_{-mi} | (123;45) \rangle \quad (3-40)$$

The differentiation on the right-hand side of eq.(3-40) is the same as that in L_{1m} .

By eq.(3-29), this reduces to

$$\begin{aligned} L_{2m} = & (-1)^m \frac{|J|^{3/2}}{4} \int [6 R Y_1^{m*}(\Omega) + 5 \vec{r}_4 Y_1^{m*}(\omega_4)] \left\{ -\frac{1}{3} R Y_1^m(\Omega) \right. \\ & - R^2 [f_1 R Y_1^m(\Omega) + f_2 \vec{r}_2 Y^m(\omega_2) + f_3 \vec{r}_3 Y^m(\omega_3) \\ & \left. + f_4 \vec{r}_4 Y_1^m(\omega_4)] \right\} \exp(-\phi') d\tau \end{aligned}$$

where

$$\begin{aligned}
 \phi' &= (A'_1 + A_2) R^2 + (B'_1 + B_2) \bar{r}_2^2 + (C'_1 + C_2) \bar{r}_3^2 + \dots \\
 &+ (K'_1 + K_2) \vec{r}_3 \cdot \vec{r}_4 \\
 &= A' R^2 + B' \bar{r}_2^2 + C' \bar{r}_3^2 + D' \bar{r}_4^2 + E' R_{cm}^2 + F' \vec{R} \cdot \vec{r}_2 \\
 &+ G' \vec{R} \cdot \vec{r}_3 + H' \vec{R} \cdot \vec{r}_4 + I' \vec{r}_2 \cdot \vec{r}_3 + J' \vec{r}_2 \cdot \vec{r}_4 + K' \vec{r}_3 \cdot \vec{r}_4
 \end{aligned}
 \tag{3-41}$$

To eliminate the cross-product terms in the quadratic form ϕ' , the transformation (3-30) will be used again. The numerical values of the coefficients (the a's) are different from those in L_{1m} . They will be denoted by a prime.

The transformed L_{2m} is

$$\begin{aligned}
 L_{2m} &= (-1)^m \frac{|J_1|^3 |J_2|^3}{4} \int [e'_1 \rho_1 Y_1^{m*}(\Omega_1) + e'_4 \rho_4 Y_1^{m*}(\Omega_4)] \\
 &\left\{ -\frac{1}{3} \rho_1^2 Y_1^m(\Omega_1) - \rho_1^2 [c'_1 \rho_1 Y_1^m(\Omega_1) + c'_2 \rho_2 Y_1^m(\Omega_2) \right. \\
 &+ c'_3 \rho_3 Y_1^m(\Omega_3) + c'_4 \rho_4 Y_1^m(\Omega_4)] \left. \right\} \exp [- (A'_0 \rho_1^2 + B' \rho_2^2 \\
 &+ C'_0 \rho_3^2 + D'_0 \rho_4^2)] d\vec{\rho}_1 d\vec{\rho}_2 d\vec{\rho}_3 d\vec{\rho}_4 e^{-E' \rho_5^2} d\vec{\rho}_5
 \end{aligned}$$

with $e'_1 = 6 + 5 a'_{41}$

$$e'_4 = 5$$

The c's and A'_0, C'_0, D'_0 have the same form as in eq.(3-33)

and (3-34), but different numerical values.

In analogy to eqs.(3-36) and (3-37),

$$\begin{aligned}
 L_{2m} = & (-1)^{m+1} \frac{|J_1|^3}{4} \int \left\{ \frac{1}{3} e_1' \rho_1^2 Y_1^{m*}(\Omega_1) Y_1^m(\Omega_1) \right. \\
 & + \rho_1^2 \left[c_4' e_4' \rho_4^2 Y_1^{m*}(\Omega_4) Y_1^m(\Omega_4) + c_1' e_1' \rho_1^2 Y_1^{m*}(\Omega_1) Y_1^m(\Omega_1) \right] \Big\} \\
 & \rho_1^2 \rho_2^2 \rho_3^2 \rho_4^2 \exp \left[- (A' \rho_1^2 + B' \rho_2^2 + C' \rho_3^2 + D' \rho_4^2) \right] \\
 & d\rho_1 d\rho_2 d\rho_3 d\rho_4 d\Omega_1 d\Omega_2 d\Omega_3 d\Omega_4 \\
 = & (-1)^{m+1} \frac{81}{4} \frac{\pi^5}{A_0'(A_0'B_0'C_0'D_0')} \left(\frac{e_1'}{3} + \frac{5 e_1' c_1'}{2 A_0'} + \frac{3 e_4' c_4'}{2 D_0'} \right)
 \end{aligned} \tag{3-42}$$

Using eqs.(3-13) and (3-9), the first part of $B_E(1)$ in eq.(3-1) can be calculated.

The expression $\langle f | K_{1m} | i \rangle$ can now be written in terms of I_0 . (Note that $I_1 = I_{-1} = -I_0$)

$$\begin{aligned}
 \langle \bar{\Phi}_f(\frac{3}{2}) | K_{1-1} | \varphi_i(\frac{1}{2}) \rangle &= - \frac{N_i N_f}{6\sqrt{2}} I_0 \\
 \langle \bar{\Phi}_f(\frac{1}{2}) | K_{10} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{6\sqrt{3}} I_0 \\
 \langle \bar{\Phi}_f(\frac{1}{2}) | K_{1-1} | \varphi_i(-\frac{1}{2}) \rangle &= - \frac{N_i N_f}{6\sqrt{6}} I_0 \\
 \langle \bar{\Phi}_f(-\frac{1}{2}) | K_{11} | \varphi_i(\frac{1}{2}) \rangle &= - \frac{N_i N_f}{6\sqrt{6}} I_0 \\
 \langle \bar{\Phi}_f(-\frac{1}{2}) | K_{10} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{6\sqrt{3}} I_0 \\
 \langle \bar{\Phi}_f(-\frac{3}{2}) | K_{11} | \varphi_i(-\frac{1}{2}) \rangle &= - \frac{N_i N_f}{6\sqrt{2}} I_0
 \end{aligned} \tag{3-43}$$

where

$$I_0 = \frac{\hbar}{mck} (L_{10} - L_{20})$$

CHAPTER IV

METHOD OF CALCULATION OF $\langle f | \vec{V} | i \rangle$

In this chapter, the second term in eq.(3-1), the matrix element of V_{1m} will be calculated. As in the case of K_{1m} , V_{1m} is related to the components of \vec{V} in a manner similar to eqs.(2-22) and (2-23), where \vec{V} is given by eq.(2-18), which is

$$\vec{V} = -i \frac{V_{LS}}{2\hbar ck} \sum_i^Z \sum_{j=1}^A v_{ij} (\vec{\sigma}_i + \vec{\sigma}_j) \times (\vec{r}_i - \vec{r}_j) \quad (4-1)$$

This operator contains spin operators and hence the complete original wave functions eq.(A-1) to (A-4) and eqs.(1-9), (1-10) must be used in calculating the matrix element, eq.(1-13).

\vec{V} can be written in terms of its components. Let

$$\vec{V} = +i \frac{V_{LS}}{2\hbar ck} \vec{U} = i \frac{V_{LS}}{2\hbar ck} (\vec{i} U_x + \vec{j} U_y + \vec{k} U_z) \quad (4-2)$$

where

$$U_x = \sum_i^Z \sum_{j=1}^A v_{ij} [(\vec{r}_i - \vec{r}_j)_y (\vec{\sigma}_i + \vec{\sigma}_j)_z - (\vec{r}_i - \vec{r}_j)_z (\vec{\sigma}_i + \vec{\sigma}_j)_y] \quad (4-3)$$

$$U_y = \sum_i^Z \sum_{j=1}^A v_{ij} [(\vec{r}_i - \vec{r}_j)_z (\vec{\sigma}_i + \vec{\sigma}_j)_x - (\vec{r}_i - \vec{r}_j)_x (\vec{\sigma}_i + \vec{\sigma}_j)_z] \quad (4-4)$$

$$U_z = \sum_i^Z \sum_{j=1}^A v_{ij} [(\vec{r}_i - \vec{r}_j)_x (\vec{\sigma}_i + \vec{\sigma}_j)_y - (\vec{r}_i - \vec{r}_j)_y (\vec{\sigma}_i + \vec{\sigma}_j)_x] \quad (4-5)$$

The subscripts denote components. The spatial operators

commute with spin operators, so their orders are immaterial.

Our problem is then reduced to evaluating the integral, eq.(1-13), with U_z , $U_x \pm i U_y$ substituted for R_{10} , $R_{1\pm 1}$, and $\varphi_i(M_i)$ substituted for $\Phi_i(M_i)$. This can be done because U_{1m} commutes with the antisymmetrization operator A , and A is hermitian and idempotent⁽³⁾.

These integrals are of the form

$$\langle \Phi_f(M_f) | U_{1m} | \varphi_i(M_i) \rangle$$

$$\text{where } U_{10} = \sqrt{\frac{3}{4\pi}} U_z \quad (4-6)$$

$$U_{1\pm 1} = \mp \sqrt{\frac{3}{8\pi}} (U_x \mp i U_y) \quad (4-7)$$

1. Matrix Element of U_{1m}

Since the spin operators change the spin coordinates when they operate on the initial state vector, the terms in eq.(1-13) must be calculated separately. Only the calculation of $\langle \Phi_f(\frac{3}{2}) | U_{1-1} | \varphi_i(\frac{1}{2}) \rangle$ is given in detail here. All other terms can be evaluated using the same method.

From eqs.(1-9) and (1-10), it is seen that the spatial part of the initial state wave function, on which U_{1m} operates, is always (123;45). Therefore, expanding the summation in eq.(4-3), U_x can be written as

$$\begin{aligned} U_x = & v_{31} \left[(z_3 - z_1)(\sigma_{3y} + \sigma_{1y}) - (y_3 - y_1)(\sigma_{3z} + \sigma_{1z}) \right] \\ & + v_{32} \left[(z_3 - z_2)(\sigma_{3y} + \sigma_{2y}) - (y_3 - y_2)(\sigma_{3z} + \sigma_{2z}) \right] \\ & + v_{34} \left[(z_3 - z_4)(\sigma_{3y} + \sigma_{4y}) - (y_3 - y_4)(\sigma_{3z} + \sigma_{4z}) \right] + \end{aligned}$$

$$\begin{aligned}
 & + v_{35} \left[(z_3 - z_5)(\sigma_{3y} + \sigma_{5y}) - (y_3 - y_5)(\sigma_{3z} + \sigma_{5z}) \right] \\
 & + v_{41} \left[(z_4 - z_1)(\sigma_{4y} + \sigma_{1y}) - (y_4 - y_1)(\sigma_{4z} + \sigma_{1z}) \right] \\
 & + v_{42} \left[(z_4 - z_2)(\sigma_{4y} + \sigma_{2y}) - (y_4 - y_2)(\sigma_{4z} + \sigma_{2z}) \right] \\
 & + v_{43} \left[(z_4 - z_3)(\sigma_{4y} + \sigma_{3y}) - (y_4 - y_3)(\sigma_{4z} + \sigma_{3z}) \right] \\
 & + v_{45} \left[(z_4 - z_5)(\sigma_{4y} + \sigma_{5y}) - (y_4 - y_5)(\sigma_{4z} + \sigma_{5z}) \right] \\
 & = P_{x31} + P_{x32} + P_{x34} + P_{x35} + P_{x41} + P_{x42} + P_{x43} + P_{x45} \quad (4-8)
 \end{aligned}$$

The P_x operators are defined by eq.(4-8), each corresponding to one bracket. Since

$$P_{x34} = - P_{x43}$$

the two terms $P_{x34} + P_{x43}$ cancel one another. Similar expressions can be written for U_y and U_z .

The summation over spin coordinates will be carried out first. The spin operators have the following properties

$$\sigma_x \alpha = \beta$$

$$\sigma_y \alpha = i\beta$$

$$\sigma_z \alpha = \alpha$$

$$\sigma_x \beta = \alpha$$

$$\sigma_y \beta = -i\alpha$$

$$\sigma_z \beta = -\beta$$

(4-9)

The initial state wave function $\varphi_i(\frac{1}{2})$ is, from eq.(1-9)

$$\begin{aligned} \varphi_i(\frac{1}{2}) = \frac{N_i}{\sqrt{18}} & (\alpha_1 \alpha_2 \beta_3 \alpha_4 \beta_5 + \alpha_1 \alpha_2 \beta_3 \beta_4 \alpha_5 + \alpha_1 \beta_2 \beta_3 \alpha_4 \alpha_5 \\ & + \beta_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 + \beta_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 + \beta_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 - 2 \alpha_1 \beta_2 \alpha_3 \alpha_4 \beta_5 \\ & - 2 \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 - 2 \beta_1 \alpha_2 \beta_3 \alpha_4 \alpha_5) \quad (123;45) \end{aligned}$$

Using eq.(4-9), and noting that spin coordinates of different particles commute, we have

$$\begin{aligned} \sigma_{1y} \varphi_i(\frac{1}{2}) = i \frac{N_i}{\sqrt{18}} & (\beta_1 \alpha_2 \beta_3 \alpha_4 \beta_5 + \beta_1 \alpha_2 \beta_3 \beta_4 \alpha_5 + \beta_1 \beta_2 \beta_3 \alpha_4 \alpha_5 \\ & - \alpha_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 - \alpha_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 - \alpha_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 - 2 \beta_1 \beta_2 \alpha_3 \alpha_4 \beta_5 \\ & - 2 \beta_1 \beta_2 \alpha_3 \beta_4 \alpha_5 + 2 \alpha_1 \alpha_2 \beta_3 \alpha_4 \alpha_5) \quad (123;45) \end{aligned}$$

$$\begin{aligned} \sigma_{2y} \varphi_i(\frac{1}{2}) = i \frac{N_i}{\sqrt{18}} & (\alpha_1 \beta_2 \beta_3 \alpha_4 \beta_5 + \alpha_1 \beta_2 \beta_3 \beta_4 \alpha_5 - \alpha_1 \alpha_2 \beta_3 \alpha_4 \beta_5 \\ & + \beta_1 \beta_2 \alpha_3 \alpha_4 \beta_5 + \beta_1 \beta_2 \alpha_3 \beta_4 \alpha_5 - \beta_1 \alpha_2 \alpha_3 \alpha_4 \alpha_5 + 2 \alpha_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 \\ & + 2 \alpha_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 - 2 \beta_1 \beta_2 \beta_3 \alpha_4 \alpha_5) \quad (123;45) \end{aligned}$$

$$\begin{aligned} \sigma_{3y} \varphi_i(\frac{1}{2}) = i \frac{N_i}{\sqrt{18}} & (-\alpha_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 - \alpha_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 - \alpha_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 \\ & + \beta_1 \alpha_2 \beta_3 \alpha_4 \beta_5 + \beta_1 \alpha_2 \beta_3 \beta_4 \alpha_5 + \beta_1 \beta_2 \beta_3 \alpha_4 \alpha_5 - 2 \alpha_1 \beta_2 \beta_3 \alpha_4 \beta_5 \\ & - 2 \alpha_1 \beta_2 \beta_3 \beta_4 \alpha_5 + 2 \beta_1 \alpha_2 \alpha_3 \alpha_4 \alpha_5) \quad (123;45) \end{aligned}$$

$$\begin{aligned} \sigma_{4y} \varphi_i(\frac{1}{2}) = i \frac{N_i}{\sqrt{18}} & (\alpha_1 \alpha_2 \beta_3 \beta_4 \beta_5 - \alpha_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 + \alpha_1 \beta_2 \beta_3 \beta_4 \alpha_5 \\ & + \beta_1 \alpha_2 \alpha_3 \beta_4 \beta_5 - \beta_1 \alpha_2 \alpha_3 \alpha_4 \alpha_5 + \beta_1 \beta_2 \alpha_3 \beta_4 \alpha_5 - 2 \alpha_1 \beta_2 \alpha_3 \beta_4 \beta_5 \\ & + 2 \alpha_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 - 2 \beta_1 \alpha_2 \beta_3 \beta_4 \alpha_5) \quad (123;45) \end{aligned}$$

$$\begin{aligned} \sigma_{5y} \varphi_i \left(\frac{1}{2} \right) &= i \frac{N_i}{\sqrt{18}} \left(-\alpha_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 + \alpha_1 \alpha_2 \beta_3 \beta_4 \beta_5 + \alpha_1 \beta_2 \beta_3 \alpha_4 \beta_5 \right. \\ &\quad - \beta_1 \alpha_2 \alpha_3 \alpha_4 \alpha_5 + \beta_1 \alpha_2 \alpha_3 \beta_4 \beta_5 + \beta_1 \beta_2 \alpha_3 \alpha_4 \beta_5 + 2 \alpha_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 \\ &\quad \left. - 2 \alpha_1 \beta_2 \alpha_3 \beta_4 \beta_5 - 2 \beta_1 \alpha_2 \beta_3 \alpha_4 \beta_5 \right) (123; 45) \end{aligned}$$

The explicit expression for $\bar{\Phi}_f \left(\frac{3}{2} \right)$ is, by eq. (A-1)

$$\begin{aligned} \bar{\Phi}_f \left(\frac{3}{2} \right) &= \frac{N_f}{12} \left(\alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 - \beta_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 - \alpha_1 \beta_2 \beta_3 \alpha_4 \alpha_5 + \beta_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 \right) (1234; 5)_1 \\ &\quad + \left(-\alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 + \alpha_1 \alpha_2 \alpha_3 \beta_4 \beta_5 + \alpha_1 \beta_2 \beta_3 \alpha_4 \alpha_5 - \alpha_1 \alpha_2 \beta_3 \alpha_4 \beta_5 \right) (5234; 1)_1 \\ &\quad + \left(\beta_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 - \alpha_1 \alpha_2 \alpha_3 \beta_4 \beta_4 - \beta_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 + \alpha_1 \alpha_2 \beta_3 \alpha_4 \right) (1534; 2)_1 \end{aligned} \quad (4-11)$$

Since each term in $\bar{\Phi}_f \left(\frac{3}{2} \right)$ has an odd number of α 's, while each term in $\sigma_{ky} \varphi_i \left(\frac{1}{2} \right)$ has an even number of α 's, by the orthogonality property of spin functions,

$$\left\langle \bar{\Phi}_f \left(\frac{3}{2} \right) \middle| \sigma_{ky} \middle| \varphi_i \left(\frac{1}{2} \right) \right\rangle = 0 \quad (4-12)$$

for $k = 1, 2, 3, 4, 5$.

The action of the z-component of $\vec{\sigma}$ on $\varphi_i \left(\frac{1}{2} \right)$ can be computed in a similar way.

$$\begin{aligned} \sigma_{1z} \varphi_i \left(\frac{1}{2} \right) &= \frac{N_i}{\sqrt{18}} \left(\alpha_1 \alpha_2 \beta_3 \alpha_4 \beta_5 + \alpha_1 \alpha_2 \beta_3 \beta_4 \alpha_5 + \alpha_1 \beta_2 \beta_3 \alpha_4 \alpha_5 \right. \\ &\quad - \beta_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 - \beta_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 - \beta_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 - 2 \alpha_1 \beta_2 \alpha_3 \alpha_4 \beta_5 \\ &\quad \left. - 2 \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 + 2 \beta_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 \right) (123; 45) \end{aligned}$$

$$\begin{aligned}
 \sigma_{2z} \varphi_i \left(\frac{1}{2}\right) &= \frac{N_i}{\sqrt{18}} \left(\alpha_1 \alpha_2 \beta_3 \alpha_4 \beta_5 + \alpha_1 \alpha_2 \beta_3 \beta_4 \alpha_5 - \alpha_1 \beta_2 \beta_3 \alpha_4 \alpha_5 \right. \\
 &\quad + \beta_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 + \beta_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 - \beta_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 + 2 \alpha_1 \beta_2 \alpha_3 \alpha_4 \beta_5 \\
 &\quad \left. + 2 \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 - 2 \beta_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 \right) (123;45) \\
 \sigma_{3z} \varphi_i \left(\frac{1}{2}\right) &= \frac{N_i}{\sqrt{18}} \left(-\alpha_1 \alpha_2 \beta_3 \alpha_4 \beta_5 - \alpha_1 \alpha_2 \beta_3 \beta_4 \alpha_5 - \alpha_1 \beta_2 \beta_3 \alpha_4 \alpha_5 \right. \\
 &\quad + \beta_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 + \beta_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 + \beta_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 - 2 \alpha_1 \beta_2 \alpha_3 \alpha_4 \beta_5 \\
 &\quad \left. - 2 \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 + 2 \beta_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 \right) (123;45) \\
 \sigma_{4z} \varphi_i \left(\frac{1}{2}\right) &= \frac{N_i}{\sqrt{18}} \left(\alpha_1 \alpha_2 \beta_3 \alpha_4 \beta_5 - \alpha_1 \alpha_2 \beta_3 \beta_4 \alpha_5 + \alpha_1 \beta_2 \beta_3 \alpha_4 \alpha_5 \right. \\
 &\quad + \beta_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 - \beta_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 + \beta_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 - 2 \alpha_1 \beta_2 \alpha_3 \alpha_4 \beta_5 \\
 &\quad \left. + 2 \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 - 2 \beta_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 \right) (123;45) \\
 \sigma_{5z} \varphi_i \left(\frac{1}{2}\right) &= \frac{N_i}{\sqrt{18}} \left(-\alpha_1 \alpha_2 \beta_3 \alpha_4 \beta_5 + \alpha_1 \alpha_2 \beta_3 \beta_4 \alpha_5 + \alpha_1 \beta_2 \beta_3 \alpha_4 \alpha_5 \right. \\
 &\quad - \beta_1 \alpha_2 \alpha_3 \alpha_4 \beta_5 + \beta_1 \alpha_2 \alpha_3 \beta_4 \alpha_5 + \beta_1 \beta_2 \alpha_3 \alpha_4 \alpha_5 + 2 \alpha_1 \beta_2 \alpha_3 \alpha_4 \beta_5 \\
 &\quad \left. - 2 \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 - 2 \beta_1 \alpha_2 \beta_3 \alpha_4 \alpha_5 \right) (123;45)
 \end{aligned} \tag{4-13}$$

Taking the scalar product of $\bar{\Phi}_f \left(\frac{3}{2}\right)$ with $\sigma_{kz} \varphi_i \left(\frac{1}{2}\right)$ and retaining only terms having the same spin configurations leads to the expressions

$$\begin{aligned}
 \langle \bar{\Phi}_f \left(\frac{3}{2}\right) | \sigma_{1z} | \varphi_i \left(\frac{1}{2}\right) \rangle &= \frac{N_i N_f}{12 \sqrt{18}} \int \left[2 (5234;1)_1 - 2 (1534;2)_1 \right] d\tau \tag{4-14} \\
 \langle \bar{\Phi}_f \left(\frac{3}{2}\right) | \sigma_{2z} | \varphi_i \left(\frac{1}{2}\right) \rangle &= \frac{N_i N_f}{12 \sqrt{18}} \int \left[-4 (5234;1)_1 + 4 (1534;2)_1 \right] d\tau
 \end{aligned}$$

$$\langle \bar{\Phi}_f(\frac{3}{2}) | \sigma_{3z} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{12\sqrt{18}} \int [2 (5234;1)_1 - 2 (1534;2)_1] d\tau$$

$$\langle \bar{\Phi}_f(\frac{3}{2}) | \sigma_{4z} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{12\sqrt{18}} \int [-2 (5234;1)_1 + 2 (1534;2)_1] d\tau$$

$$\langle \bar{\Phi}_f(\frac{3}{2}) | \sigma_{5z} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{12\sqrt{18}} \int [-6 (1234;5)_1 + 4 (5234;1)_1 + 2 (1534;2)_1] d\tau$$

An expression for U_y similar to eq.(4-8) can be written symbolically as

$$U_y = P_{y31} + P_{y32} + P_{y35} + P_{y41} + P_{y42} + P_{y45} \quad (4-15)$$

It can be shown that the action of σ_{kx} on $\varphi_i(\frac{1}{2})$ gives an expression with each term having an even number of α 's.

Therefore, by the same argument as in σ_{ky}

$$\langle \bar{\Phi}_f(\frac{3}{2}) | \sigma_{ky} | \varphi_i(\frac{1}{2}) \rangle = 0, \quad k = 1, 2, 3, 4, 5$$

Combining eqs.(4-80), (4-14), (4-15) yields

$$\begin{aligned} \langle \bar{\Phi}_f(\frac{3}{2}) | U_{1-1} | \varphi_i(\frac{1}{2}) \rangle &= \sqrt{\frac{3}{8\pi}} \langle \bar{\Phi}_f(\frac{3}{2}) | U_x + i U_y | \varphi_i(\frac{1}{2}) \rangle \\ &= i \sqrt{\frac{3}{8\pi}} \frac{N_i N_f}{12\sqrt{18}} \int \left\{ \left[6 v_{35}(x_3 - iy_3) + 6 v_{45}(x_4 - iy_4) \right. \right. \\ &\quad \left. \left. + (-6 v_{35} - 6 v_{45})(x_5 - iy_5) \right] (1234;5)_1^* \right. \\ &\quad \left. + \left[4v_{13}(x_1 + iy_1) + (-2v_{23} - 6v_{24})(x_2 + iy_2) + (-4v_{13} + 2v_{23} - 6v_{35}) \right. \right. \\ &\quad \left. \left. (x_3 + iy_3) + (6v_{24} - 2v_{45})(x_4 + iy_4) + (6v_{35} + 2v_{45})(x_5 + iy_5) \right] (5234;1)_1^* \right\} \end{aligned}$$

$$\begin{aligned}
 & + \left[-4v_{13}(x_1+iy_1) + (2v_{23}+6v_{24})(x_2+iy_2) + (4v_{13}-2v_{23})(x_3+iy_3) \right. \\
 & \left. + (-6v_{24}-4v_{45})(x_4+iy_4) + 4v_{45}(x_5+iy_5) \right] (1534;2)_1^* \int (123;45) d\tau \\
 & = -i \frac{N_i N_f}{12\sqrt{18}} M_1(x+iy) \tag{4-16}
 \end{aligned}$$

where $M_1(x+iy)$ stands for the integral, the subscript 1 denoting $M_f=1$ for the final state spatial wave function, and $(x+iy)$ denoting the fact that the dependence of M_1 on the x and y is always of this form.

This integral can be evaluated by using a method similar to that used in evaluating L_{1m} given on page 27. The detailed calculation will be given later.

We have now summed over the spin coordinates of the first term in eq.(1-13). The other term can also be expressed in an integral form in exactly the same manner. The second term of eq.(1-13) is

$$\langle \bar{\Phi}_f(\frac{1}{2}) | U_{10} | \varphi_i(\frac{1}{2}) \rangle = \sqrt{\frac{3}{4\pi}} \langle \bar{\Phi}_f(\frac{1}{2}) | U_z | \varphi_i(\frac{1}{2}) \rangle \tag{4-17}$$

where

$$U_z = P_{z31} + P_{z32} + P_{z35} + P_{z41} + P_{z42} + P_{z45} \tag{4-18}$$

and $\bar{\Phi}_f(\frac{1}{2})$ is given by eq.(A-2).

It is seen from eq.(4-13) that each term in $\sigma_{kz} \varphi_i(\frac{1}{2})$ has an odd number of α 's, whereas $\bar{\Phi}_f(\frac{1}{2})$ has an even number of

α 's. Therefore,

$$\langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{kz} | \varphi_i(\frac{1}{2}) \rangle = 0 \quad (k = 1, 2, 3, 4, 5)$$

For the x and y components, it can be shown that

$$\begin{aligned} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{1x} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{12\sqrt{3}\sqrt{18}} \left[(1234;5)_1 + 2(5234;1)_1 - 3(1534;2)_1 \right] \\ &= \frac{1}{i} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{1y} | \varphi_i(\frac{1}{2}) \rangle \end{aligned}$$

$$\begin{aligned} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{2x} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{12\sqrt{3}\sqrt{18}} \left[-(1234;5)_1 - 3(5234;1)_1 + 4(1534;2)_1 \right] \\ &= \frac{1}{i} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{2y} | \varphi_i(\frac{1}{2}) \rangle \end{aligned}$$

$$\begin{aligned} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{3x} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{12\sqrt{3}\sqrt{18}} \left[3(1234;5)_1 - 3(1534;2)_1 \right] \\ &= \frac{1}{i} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{3y} | \varphi_i(\frac{1}{2}) \rangle \end{aligned}$$

$$\begin{aligned} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{4x} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{12\sqrt{3}\sqrt{18}} \left[-3(1234;5)_1 + 3(1534;2)_1 \right] \\ &= \frac{1}{i} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{4y} | \varphi_i(\frac{1}{2}) \rangle \end{aligned}$$

$$\begin{aligned} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{5x} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{12\sqrt{3}\sqrt{18}} \left[-6(1234;5)_1 + 3(5234;1)_1 + 3(1534;2)_1 \right] \\ &= \frac{1}{i} \langle \bar{\Phi}_f(\frac{1}{2}) | \sigma_{5y} | \varphi_i(\frac{1}{2}) \rangle \end{aligned}$$

(4-19)

Then,

$$\langle \bar{\Phi}_f(\frac{1}{2}) | u_{10} | \varphi_i(\frac{1}{2}) \rangle =$$

$$\begin{aligned}
 &= i \sqrt{\frac{3}{4\pi}} \frac{N_i N_f}{12\sqrt{3}\sqrt{18}} \left\{ \int \left[(-4v_{13} + 2v_{14})(x_1 + iy_1) + (-2v_{23} + 4v_{24})(x_2 + iy_2) \right. \right. \\
 &\quad + (4v_{13} + 2v_{23} - 3v_{35})(x_3 + iy_3) + (-2v_{14} - 4v_{24} - 9v_{45})(x_4 + iy_4) \\
 &\quad \left. \left. + (3v_{35} + 9v_{45})(x_5 + iy_5) \right] (1234; 5)_1^* (123; 45) d\tau \right. \\
 &\quad + \int \left[(-2v_{13} - 2v_{14})(x_1 + iy_1) + (3v_{23} + 3v_{24})(x_2 + iy_2) + (2v_{13} - 3v_{23} + v_{35}) \right. \\
 &\quad \left. (x_3 + iy_3) + (2v_{14} - 3v_{24} + 3v_{45})(x_4 + iy_4) + (-3v_{35} - 3v_{45})(x_5 + iy_5) \right] \\
 &\quad (5234; 1)_1^* (123; 45) d\tau \\
 &\quad + \int \left[6v_{13}(x_1 + iy_1) + (-v_{23} - 7v_{24})(x_2 + iy_2) + (-6v_{13} + v_{23})(x_3 + iy_3) \right. \\
 &\quad \left. + (7v_{24} + 6v_{45})(x_4 + iy_4) - 6v_{45}(x_5 + iy_5) \right] (1534; 2)_1^* (123; 45) d\tau \left. \right\} \\
 &= i \sqrt{\frac{3}{4\pi}} \frac{N_i N_f}{12\sqrt{3}\sqrt{18}} N_1(x+iy) \tag{4-20}
 \end{aligned}$$

where the subscript and the parenthesis in N has the same meaning as the M in eq.(4-16).

Similarly, it can be shown that

$$\langle \bar{\Phi}_f(-\frac{1}{2}) | U_{10} | \varphi_i(-\frac{1}{2}) \rangle = -i \sqrt{\frac{3}{4\pi}} \frac{N_i N_f}{12\sqrt{3}\sqrt{18}} N_{-1}(x-iy) \tag{4-21}$$

$$\langle \bar{\Phi}_f(-\frac{3}{2}) | U_{11} | \varphi_i(-\frac{1}{2}) \rangle = i \sqrt{\frac{3}{8\pi}} \frac{N_i N_f}{12\sqrt{18}} M_{-1}(x-iy) \tag{4-22}$$

$$\langle \bar{\Phi}_f(\frac{1}{2}) | U_{1-1} | \varphi_i(-\frac{1}{2}) \rangle = i \sqrt{\frac{3}{8\pi}} \frac{N_i N_f}{12\sqrt{18}} \left[M_1(x+iy) + 2\sqrt{\frac{2}{3}} N_0(z) \right] \tag{4-23}$$

$$\langle \bar{\Phi}_f(-\frac{1}{2}) | U_{11} | \varphi_i(\frac{1}{2}) \rangle = -i \sqrt{\frac{3}{8\pi}} \frac{N_i N_f}{12\sqrt{18}} \left[M_{-1}(x-iy) - 2\sqrt{\frac{2}{3}} N_0(z) \right] \tag{4-24}$$

2. Evaluation of N and M

From the last section, we see that there are five integrals involved: $N_1(x+iy)$, $N_{-1}(x-iy)$, $N_0(z)$, $M_1(x+iy)$ and $M_{-1}(x-iy)$.

Let

$$N_1(x+iy) = N_1^{(1)} + N_1^{(2)} + N_1^{(3)} \quad (4-25)$$

Each term on the right hand side of eq.(4-25) is equal to one integral in eq.(4-20), i.e.

$$\begin{aligned} N_1^{(1)} = & \int \left[4e^{-\lambda r_{13}^2} (x_3+iy_3-x_1-iy_1) + 2e^{-\lambda r_{13}^2} (x_3+iy_3-x_2-iy_2) \right. \\ & - 3e^{-\lambda r_{35}^2} (x_3+iy_3-x_5-iy_5) - 2e^{-\lambda r_{14}^2} (x_4+iy_4-x_1-iy_1) \\ & \left. - 4e^{-\lambda r_{14}^2} (x_4+iy_4-x_2-iy_2) - 9e^{-\lambda r_{45}^2} (x_4+iy_4-x_5-iy_5) \right] \\ & \cdot (1234;5)_1^* (123;45) d\tau \end{aligned} \quad (4-26)$$

In this equation, $e^{-\lambda r_{ij}^2}$ has been substituted for v_{ij} and the terms have been rearranged. Similar expressions can be written for $N_1^{(2)}$ and $N_1^{(3)}$.

Let $S_m^{(n)}(ij)$ denote an integral of the form

$$S_m^{(n)}(ij) = \int e^{-\lambda r_{ij}^2} (x_i+iy_i-x_j-iy_j) (n)_m^* (123;45) d\tau$$

where $n = 1, 2, 3$

$m = 0, \pm 1$

$i, j = 1, 2, 3, 4, 5$.

$(n)_m$ stands for the final state wave function, where $n = 1, 2, 3$ represent $(1234;5)$, $(5234;1)$ and $(1534;2)$

respectively.

Using this notation, $N_1^{(1)}$, $N_1^{(2)}$, $N_1^{(3)}$ can be written as follows

$$N_1^{(1)} = 4S_1^{(1)}(31) + 2S_1^{(1)}(32) - 3S_1^{(1)}(35) - 2S_1^{(1)}(41) - 4S_1^{(1)}(42) - 9S_1^{(1)}(45) \quad (4-27)$$

$$N_1^{(2)} = 2S_1^{(2)}(31) - 3S_1^{(2)}(32) + 3S_1^{(2)}(35) + 2S_1^{(2)}(41) - 3S_1^{(2)}(42) + 3S_1^{(2)}(45) \quad (4-28)$$

$$N_1^{(3)} = -6S_1^{(3)}(31) + S_1^{(3)}(32) + 7S_1^{(3)}(42) + 6S_1^{(3)}(45) \quad (4-29)$$

The quantities M_1 can also be written in terms of integrals of the form S .

$$M_1(x+iy) = M_1^{(1)} + M_1^{(2)} + M_1^{(3)}$$

$$M_1^{(1)} = -6S_1^{(1)}(35) - 6S_1^{(1)}(45) \quad (4-30)$$

$$M_1^{(2)} = 4S_1^{(2)}(31) - 2S_1^{(2)}(32) + 6S_1^{(2)}(35) - 6S_1^{(2)}(42) + 2S_1^{(2)}(45) \quad (4-31)$$

$$M_1^{(3)} = -4S_1^{(3)}(31) + 2S_1^{(3)}(32) + 6S_1^{(3)}(42) + 4S_1^{(3)}(45) \quad (4-32)$$

The problem is solved when the 18 integrals of the form S are evaluated. The method to evaluate $S_1^{(n)}(ij)$ is given in Appendix E.

It is also proved in Appendix E that

$$N_{-1}(x-iy) = -N_1(x+iy)$$

$$M_{-1}(x-iy) = -M_1(x+iy)$$

$$N_0(z) = -\frac{1}{\sqrt{2}} N_1(x+iy)$$

In terms of N ($= N_1(x+iy)$) and M ($= M_1(x+iy)$), eqs.(4-16), (4-20) to (4-24) can be written as

$$\begin{aligned} \langle \bar{\Phi}_f(\frac{3}{2}) | U_{1-1} | \varphi_i(\frac{1}{2}) \rangle &= + i \sqrt{\frac{3}{8\pi}} \frac{N_i N_f}{12\sqrt{18}} M \\ \langle \bar{\Phi}_f(\frac{1}{2}) | U_{10} | \varphi_i(\frac{1}{2}) \rangle &= -i \sqrt{\frac{3}{4\pi}} \frac{N_i N_f}{12\sqrt{18}} N \\ \langle \bar{\Phi}_f(-\frac{1}{2}) | U_{10} | \varphi_i(\frac{1}{2}) \rangle &= -i \sqrt{\frac{3}{4\pi}} \frac{N_i N_f}{12\sqrt{18}} N \\ \langle \bar{\Phi}_f(-\frac{3}{2}) | U_{11} | \varphi_i(\frac{1}{2}) \rangle &= + i \sqrt{\frac{3}{8\pi}} \frac{N_i N_f}{12\sqrt{18}} M \\ \langle \bar{\Phi}_f(\frac{1}{2}) | U_{1-1} | \varphi_i(\frac{1}{2}) \rangle &= -i \sqrt{\frac{3}{8\pi}} \frac{N_i N_f}{12\sqrt{18}} (M - \frac{2}{\sqrt{3}} N) \\ \langle \bar{\Phi}_f(-\frac{1}{2}) | U_{11} | \varphi_i(\frac{1}{2}) \rangle &= -i \sqrt{\frac{3}{8\pi}} \frac{N_i N_f}{12\sqrt{18}} (M - \frac{2}{\sqrt{3}} N) \end{aligned} \tag{4-33}$$

Combining eqs.(3-43) and (4-33), we have

$$\begin{aligned} \langle \bar{\Phi}_f(\frac{3}{2}) | R_{1-1} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{6\sqrt{2}} \left(-I_0 + \sqrt{\frac{3}{8\pi}} \frac{V_{LS}}{12 \hbar c k} M \right) \\ \langle \bar{\Phi}_f(\frac{3}{2}) | R_{10} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{6\sqrt{3}} \left(I_0 - \sqrt{\frac{3}{8\pi}} \frac{V_{LS}}{4\sqrt{3} \hbar c k} N \right) \\ \langle \bar{\Phi}_f(-\frac{1}{2}) | R_{10} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{6\sqrt{3}} \left(I_0 - \sqrt{\frac{3}{8\pi}} \frac{V_{LS}}{4\sqrt{3} \hbar c k} N \right) \\ \langle \bar{\Phi}_f(-\frac{3}{2}) | R_{11} | \varphi_i(\frac{1}{2}) \rangle &= \frac{N_i N_f}{6\sqrt{2}} \left(-I_0 + \sqrt{\frac{3}{8\pi}} \frac{V_{LS}}{12 \hbar c k} M \right) \end{aligned} \tag{4-34}$$

$$\langle \bar{\Phi}_f(\frac{1}{2}) | R_{1-1} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{6\sqrt{6}} \left[-I_0 - \sqrt{\frac{3}{8\pi}} \frac{V_{LS}}{4\sqrt{3} \hbar c k} (M - \frac{2}{\sqrt{3}} N) \right]$$

$$\langle \bar{\Phi}_f(\frac{1}{2}) | R_{11} | \varphi_i(\frac{1}{2}) \rangle = \frac{N_i N_f}{6\sqrt{6}} \left[-I_0 - \sqrt{\frac{3}{8\pi}} \frac{V_{LS}}{4\sqrt{3} \hbar c k} (M - \frac{2}{\sqrt{3}} N) \right]$$

CHAPTER V

NUMERICAL CALCULATION

The explicit form for the transition probability has been worked out in previous chapters. The equations needed for its calculation are summarized here.

The E1 transition probability is given by

$$T_E(1) = \frac{16\pi k^3}{9} \frac{e^2}{\hbar} \frac{1}{4} B_E(1) \quad (5-1)$$

where

$$\begin{aligned} B_E(1) = & \left| \langle \bar{\Phi}_f(\frac{3}{2}) | R_{1-1} | \varphi_i(\frac{1}{2}) \rangle \right|^2 + \left| \langle \bar{\Phi}_f(\frac{3}{2}) | R_{10} | \varphi_i(\frac{1}{2}) \rangle \right|^2 \\ & + \left| \langle \bar{\Phi}_f(\frac{1}{2}) | R_{1-1} | \varphi_i(-\frac{1}{2}) \rangle \right|^2 + \left| \langle \bar{\Phi}_f(-\frac{1}{2}) | R_{11} | \varphi_i(\frac{1}{2}) \rangle \right|^2 \\ & + \left| \langle \bar{\Phi}_f(-\frac{1}{2}) | R_{10} | \varphi_i(-\frac{1}{2}) \rangle \right|^2 + \left| \langle \bar{\Phi}_f(-\frac{3}{2}) | R_{11} | \varphi_i(-\frac{1}{2}) \rangle \right|^2 \end{aligned} \quad (5-2)$$

Each term is expressed in terms of I_0 , M and N by eq.(4-44).

The problem is now reduced to the evaluation of I_0 , M and N . I_0 is given by

$$I_0 = \frac{\hbar}{mck} (L_{10} - L_{20}) \quad (5-3)$$

where

$$\begin{aligned} L_{10} = & -\frac{81}{4} \frac{\pi^5}{A_0 (A_0 B C_0 D_0)^{3/2}} \left(\frac{e_1}{3A_0} + \frac{5e_1 c_1}{2A_0} + \frac{3e_2 c_2}{2B} \right. \\ & \left. + \frac{3e_3 c_3}{2C_0} + \frac{3e_4 c_4}{2D_0} \right) \end{aligned} \quad (5-4)$$

and

$$L_{20} = -\frac{81}{4} \frac{\pi^5}{A_0'(A_1^2 B_1^2 C_1^2 D_1^2)} \left(\frac{e_1^4}{2A_1^2} + \frac{5e_1^2 c_1^2}{2B_1^2} + \frac{3e_1^2 c_1^2}{2D_1^2} \right) \quad (5-5)$$

The constants are given in terms of the variational parameters $\alpha, \bar{\alpha}, \beta, \alpha_1,$ and β_1 .

$$N = N_1^{(1)} + N_1^{(2)} + N_1^{(3)} \quad (5-6)$$

$$M = M_1^{(1)} + M_1^{(2)} + M_1^{(3)} \quad (5-7)$$

Here the $M_1^{(n)}$'s and $N_1^{(n)}$'s can be written as linear combinations of $S_1^{(n)}(ij)$ as in eqs. (4-27) to (4-32); $S_1^{(n)}(ij)$ is of the form

$$S_1^{(n)}(ij) = -\sqrt{\frac{8\pi}{3}} \frac{81\pi^5}{8} \frac{1}{A_0''(A_0''B''C_0''D_0'')^{3/2}} \left(\frac{5c_{11}}{A_0''} + \frac{3c_{22}}{B''} + \frac{3c_{33}}{C_0''} + \frac{3c_{44}}{D_0''} \right) \quad (5-8)$$

For each different set of $n, (ij)$, there is different set of values of the constants $A_0'', B'', C_0'', D_0'', c_{11}, c_{22}, c_{33}$ and c_{44} . n assumes the values 1, 2 and 3, and (ij) assumes the values (31), (32), (35), (41), (42) and (45). Therefore, there are 18 separate $S_1^{(n)}(ij)$ which must be calculated.

Before carrying out this calculation, some constants which are known or have been calculated are listed here (2)(3).

The variational parameters in the wave functions are

$$\alpha = 2.81 \times 10^{25} \text{ cm}^{-2}$$

$$\bar{\alpha} = 4.78 \times 10^{25} \text{ cm}^{-2}$$

$$\beta = 0.422 \times 10^{25} \text{ cm}^{-2}$$

$$\alpha_1 = 4.33 \times 10^{25} \text{ cm}^{-2}$$

$$\beta' = \left\{ \begin{array}{l} 2.25 \\ 3.25 \end{array} \right\} \times 10^{25} \text{ cm}^{-2}$$

The range (λ) and depth (V_{LS}) of the spin orbit potential in eq.(2-10) are

$$\lambda = \left\{ \begin{array}{l} 2.657 \\ 4.16 \end{array} \right\} \times 10^{25} \text{ cm}^{-2}$$

$$V_{LS} = \left\{ \begin{array}{l} 4.5 \\ 13.5 \end{array} \right\} \text{ Mev}$$

The squares of the normalization constants have been computed to be (3)

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

$$N_f^2 = \left\{ \begin{array}{l} 3.50 \\ 8.45 \end{array} \right\} \times 10^{176} \text{ cm}^{-14}$$

The wave number is

$$k = \frac{\Delta E}{\hbar c} = 8.45 \times 10^{11} \text{ cm}^{-1}$$

ΔE being the energy difference of the two states.

Some of the above constants are given two different values; this results from two different

choices of the range and depth of the spin-orbit potential⁽²⁾; both give good agreement with the energy levels of the two states. Therefore, there will be two values for each quantity in the following calculations.

The numerical values of the constants in eqs.(5-4) and (5-5) are given in Appendix D. Inserting these values into the two equations leads to the results:

$$L_{10} = \left\{ \begin{array}{l} -0.437 \\ -0.228 \end{array} \right\} \times 10^{-175} \text{ cm}^{14}$$

$$L_{20} = \left\{ \begin{array}{l} -1.214 \\ -0.649 \end{array} \right\} \times 10^{-175} \text{ cm}^{14}$$

and by eq.(5-3),

$$I_0 = \left\{ \begin{array}{l} 1.924 \\ 1.043 \end{array} \right\} \times 10^{-201} \text{ cm}^{16}$$

The 18 sets of values of the constants in eq.(5-8) are given in Appendix F. Making use of eqs.(4-27) to (4-32), we obtain

$$M_1^{(1)} = \left\{ \begin{array}{l} 11.725 \\ 3.386 \end{array} \right\} \times 10^{199} \text{ cm}^{16}$$

$$M_1^{(2)} = \left\{ \begin{array}{l} 1.427 \\ 0.118 \end{array} \right\} \times 10^{199} \text{ cm}^{16}$$

$$M_1^{(3)} = \begin{Bmatrix} -8.080 \\ -5.263 \end{Bmatrix} \times 10^{199} \text{ cm}^{16}$$

$$N_1^{(1)} = \begin{Bmatrix} 9.230 \\ 2.760 \end{Bmatrix} \times 10^{199} \text{ cm}^{16}$$

$$N_1^{(2)} = \begin{Bmatrix} -6.222 \\ -4.964 \end{Bmatrix} \times 10^{199} \text{ cm}^{16}$$

$$N_1^{(3)} = \begin{Bmatrix} 21.453 \\ -22.638 \end{Bmatrix} \times 10^{199} \text{ cm}^{16}$$

$$M = M_1^{(1)} + M_1^{(2)} + M_1^{(3)} = \begin{Bmatrix} 5.072 \\ -1.762 \end{Bmatrix} \times 10^{199} \text{ cm}^{16}$$

$$N = N_1^{(1)} + N_1^{(2)} + N_1^{(3)} = \begin{Bmatrix} 24.463 \\ -24.838 \end{Bmatrix} \times 10^{199} \text{ cm}^{16}$$

Substituting the values of I_0 , M and N into eqs.(4-34) and (5-2), we obtain

$$B_E(1) = \begin{Bmatrix} 2.129 \\ 1.754 \end{Bmatrix} \times 10^{-29} \text{ cm}^2$$

By eq.(5-1), the transition probability is therefore

$$T_E(1) = \begin{Bmatrix} 3.96 \\ 3.26 \end{Bmatrix} \times 10^{15} \text{ sec}^{-1}$$

The level width Γ_r for the transition is related to the transition probability by

$$\Gamma_r = \hbar T_E(1)$$

or numerically

$$\Gamma_r = 0.658 \times 10^{-15} T_{\beta}(1) \text{ ev} ,$$

so

$$\Gamma_r = \begin{cases} 2.61 & \text{ev} \\ 2.15 & \text{ev} \end{cases}$$

CHAPTER VI

CONCLUSION

For the transition between these two energy levels, no experiment has ever been performed to measure directly the width of the $3/2 +$ level. However, the width can be deduced from experiments on the $T(d, \gamma)He^5$ and $T(d, n)He^4$ reactions (7)(8).

It is known⁽⁴⁾ that the radiative width is approximately

$$\Gamma_{\gamma} \approx 1.3 \text{ ev}$$

Comparing this value with the calculated values, it is seen that the latter are about two times larger than the experimental value, and are also larger than the values calculated by using the conventional operator \hat{T} (see Table 1). However, it is still far better than the prediction of the single particle model⁽³⁾⁽⁴⁾.

Experimental value	Theory (Tran Duc)	Theory (This work)	Theory (Single particle model)
1.32 ev	1.23 ev 1.12 ev	2.65 ev 2.15 ev	184.8 ev

Table 1. Radiative Width of the $3/2 +$ Level in the He^5 Nucleus

It is apparent that the cluster model provides a better description of the He^5 nucleus than does the single particle model. However, the single particle model is itself a very poor model due to the many approximations and assumptions involved in its formulation. A more realistic model which does not assume clustering features in the nucleus is the shell model. It has been shown by Wilkinson⁽¹²⁾ that the distribution of E1 transition matrix elements of light nuclei is consistent with shell model expectations. But, as indicated in the same paper, from the observed transitions of higher multiplicities in light nuclei, there seems to be clear indications of collective behaviour in nuclear structure, and this can be taken as implying that some clustering actually occurs in these nuclei.

As has been shown by Bethe and Salpeter⁽⁹⁾, in calculations of atomic transition probabilities, the operator \vec{r} is preferred when the wave function is important at distances far from the centre of mass, while $\frac{\hbar}{m\omega} \vec{\nabla}$ is preferred if the wave function is important at intermediate distances. In other words, \vec{r} can test the correctness of the wave function in a region far from the centre of mass, while $\frac{\hbar}{m\omega} \vec{\nabla}$ tests the correctness of the wave function in a region close to the centre of mass.

Chandrasekhar⁽¹⁰⁾ used these two methods for transitions from the ground state to states in the continuum of the

H^- -ion. His results justified the above statement. In the case of nuclear radiative transitions, this statement is still valid, because, as can be seen in Chapter II, the replacement of one operator by the others involves only quantum mechanical considerations, and is independent of the system to which it is applied.

Although in this work, \bar{F} is replaced by a gradient operator and an operator containing spins, the former contributes most to the results; therefore, we shall neglect the latter in the following discussion. The relative unimportance of the second term can most clearly be seen by noting that if it is neglected in eqs.(4-34) (i.e. if the explicit spin-orbit term is neglected), the level widths are found to be 2.68 ev or 1.90 ev, as compared to the total level widths 2.61 ev or 2.15 ev.

The wave functions used in the previous chapters do not assume a saturation character for the nuclear force; two nucleons can get closer than the diameter of the hard core of the nuclear force. Experimental evidence indicates that the hard core does exist, and wave functions must vanish at and within the hard core. The radius of this core is known to be approximately 0.4×10^{-13} cm, a distance which is comparable to the root mean square values of the radii of the cluster wave functions (which are 1.5×10^{-13} cm, 1.8×10^{-13} cm and 1.4×10^{-13} cm for the

α particle, triton, and deuteron respectively). That this effect is not negligible can be seen as follows.

The wave function of the relative motion of two nucleons in a Fermi gas which interact through a square well potential with hard core has been investigated by Gomes, Walecka and Weisskopf⁽¹¹⁾, who obtained the s-state ($l = 0$) solution for two distinguishable particles. The radial part of the wave function for the relative motion of the two particles for the case of no interaction (b) and for the case with interaction (a) are shown in Fig.6-1.

The potential which is used in the cluster model is a simple harmonic oscillator potential. Suppose for simplicity that all particles in the nucleus are distinguishable and move in a common oscillator potential well. From the fact that the form of the wave function of a single particle does not change appreciably between a simple harmonic oscillator, a square well and an infinite square well potential, and the situation that particles in an infinite square well potential are equivalent to non-interacting particles in a box, we infer that the average form of the pair wave function for a non-identical s-state pair in the clusters has roughly the same behaviour as curve (b) in Fig.6-1. However, in the treatment by Gomes et al., the nucleons are considered to be in an infinite nucleus and form a Fermi gas. But in the He^5 nucleus, there are only five nucleons and these hardly constitute a Fermi gas.

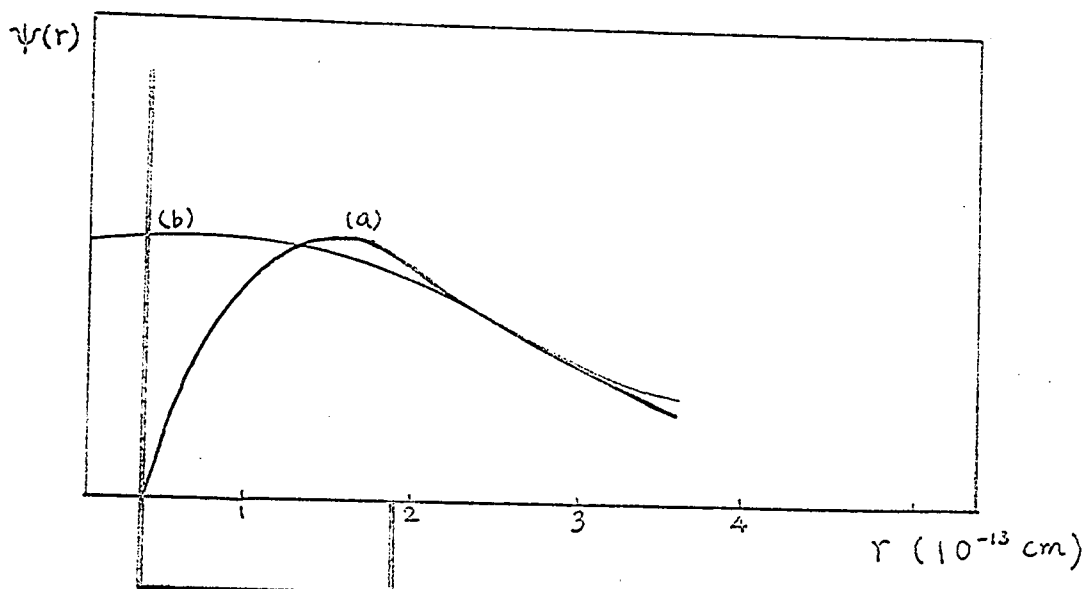


Fig.6-1. The wave function of the relative motion of two particles embedded in a Fermi gas with (a) and without (b) interaction. The heavy line shows the interaction potential. (taken from L.C. Gomes et al. *Annals of Physics* 3, 241 (1958))

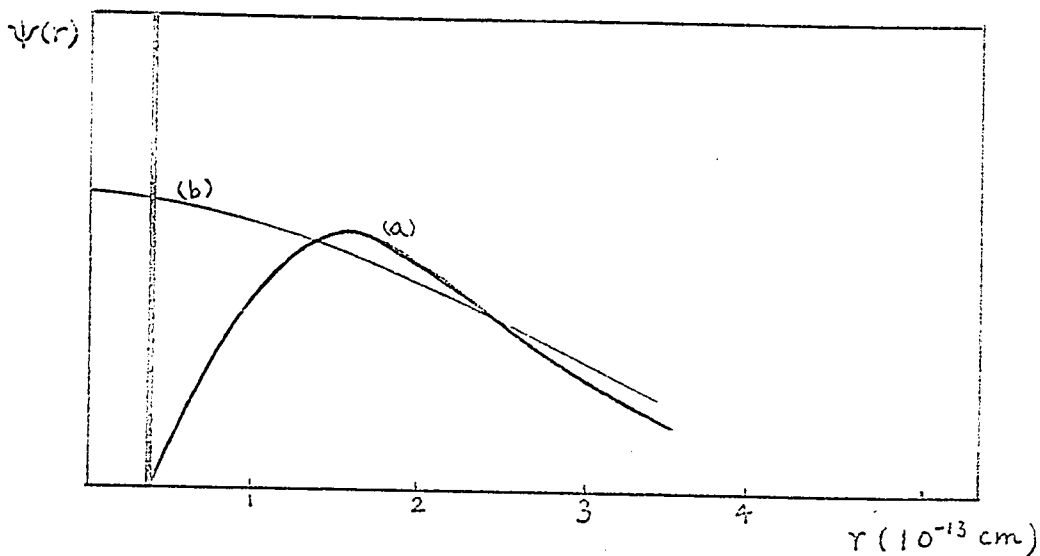


Fig.6-2. The pair wave function for a realistic nucleus (a) and for the case assuming cluster model (b). The heavy line indicates the position of the hard core of the nuclear force.

As pointed out in the same article, for very small distances ($r \ll \lambda_F$, where λ_F is the Fermi wavelength and $\lambda_F \approx 0.67 \cdot 10^{-13}$ cm), the pair wave function in a Fermi gas is equal to the pair wave function of the isolated pair. Therefore, the pair wave function of the cluster model is approximately equal to curve (b) in Fig.6-1 at $r = 0$, and will not deviate much from it for $r < \lambda_F$.

For pairs of higher orbital angular momentum, which correspond to pairs from different clusters, it is shown in the same article that the wave function is practically equal to that without interaction. For pairs of identical particles with anti-parallel spins, the probability that they coincide is large due to the effect of antisymmetrization. For pairs with parallel spins, the two particles interact as if there were a repulsive force between them. In both energy states of the He^5 nucleus, the number of attractive pairs is greater than the number of repulsive pairs; we expect that the amplitude of the average cluster model pair wave function at $r = 0$ will be larger than that of curve (b) in Fig.6-1. This is the case for the wave function which we have been using in this work.

In a realistic nucleus, the saturation character and the attractive nature of the nuclear force do exist. The general features of the average pair wave function would not deviate much from curve (a) in Fig.6-1 for small r . To compare the two cases, a probable form of the pair wave function for a

realistic nucleus (a) and for the case assuming cluster model (b) are shown in Fig.6-2.

It has been shown that the contribution to the transition probability obtained in this calculation results predominantly from a relatively small region in space. If the volume of the nucleus is small, the average distance between the nucleons is also small. Therefore, the part of the integration region in Fig.6-2 in which r is small contributes a major part of the integral. In this region, the wave function used in this work (b) is larger than the realistic one (a), and since the transition probability is proportional to the square of the matrix element, a high value for transition probability is obtained.

In Tran Duc's calculation, since the wave function at large distances from the centre of mass is more important, the region of large r in Fig.6-2 contributes a major part of the matrix element. The results he obtained are quite close to the experimental value. This fact indicates that the cluster model wave functions are good at large distances from the centre of mass of the nucleus, but not so good at small distances because the effect of the hard core of the nuclear force is neglected.

To take the effect of the hard core into account, we can multiply the wave function by a factor of the form⁽¹⁾

$$\prod_{\substack{\text{all} \\ \text{pairs}}} R(|\vec{r}_i - \vec{r}_k|)$$

where K is a function which vanishes when $|\vec{r}_i - \vec{r}_k|$ is smaller than the diameter of the hard core and approaches one asymptotically. Calculations on wave functions involving this factor are much more difficult.

Because of the large difference between the results using the two methods of calculation, and the relatively small difference between the values using different parameters, it is difficult to judge which set of parameters is more favourable to describe the nucleus.

In spite of these shortcomings, the general feature of clustering in light nuclei is still a reasonable assumption for the behaviour of the nucleus, as can be seen by comparing the values for the transition probability by using the single particle model and the cluster model. The cluster model is especially appropriate to describe qualitatively problems in nuclear physics where calculations are impossible⁽¹⁵⁾.

From the foregoing discussion, it can be seen that for theoretical calculations of the nuclear properties, the cluster model wave function will give a good result if the operators in the matrix elements are such that the contribution from large distances from the centre of mass is more important than from small distances.

It has been recently reported⁽¹³⁾ that the radiative transition from the $3/2 +$ to the $1/2 -$ state in Li^5 nucleus has been observed; a similar transition in He^5 has not yet been

observed. The parameters of the wave function of the $1/2 -$ state of He^5 cannot be obtained by a variational calculation of the energy of this state⁽²⁾. The calculated value of the radiative transition probability from the $3/2 +$ to the $3/2 -$ state (using the conventional operator $\sum_p c \frac{z}{r_p}$) agrees quite well with experiment. There is therefore some justification for using such a calculation for the $3/2 + \rightarrow 1/2 -$ transition for determining a suitable set of parameters for the $1/2 -$ state of He^5 .

APPENDIX A

The Complete Antisymmetrized
Wave Functions of the Ground State

The antisymmetrized ground state cluster model wave functions for He^5 are given by Tran Duc (3), and are

$$\begin{aligned} \bar{\Phi}_f\left(\frac{3}{2}\right) &= \frac{N_f}{3!2!} (\alpha_3\beta_4 - \beta_3\alpha_4) [(\alpha_1\beta_2 - \beta_1\alpha_2) \alpha_5 (1234;5), \\ &\quad - \alpha_1 (\beta_2\alpha_5 - \alpha_2\beta_5) (5234;1), + \alpha_2 (\beta_1\alpha_5 - \alpha_1\beta_5) (1534;2),] \\ &\hspace{20em} (A-1) \end{aligned}$$

$$\begin{aligned} \bar{\Phi}_f\left(\frac{1}{2}\right) &= \frac{N_f}{3!2!\sqrt{3}} (\alpha_3\beta_4 - \beta_3\alpha_4) \{ [(\alpha_1\beta_2 - \beta_1\alpha_2) \beta_5 (1234;5), \\ &\quad - \beta_1 (\beta_2\alpha_5 - \alpha_2\beta_5) (5234;1), + \beta_2 (\beta_1\alpha_5 - \alpha_1\beta_5) (1534;2),] \\ &\quad + \sqrt{2} [(\alpha_1\beta_2 - \beta_1\alpha_2) \alpha_5 (1234;5)_0 - \alpha_1 (\beta_2\alpha_5 - \alpha_2\beta_5) (5234;1)_0 \\ &\quad - \alpha_2 (\alpha_1\beta_5 - \beta_1\alpha_5) (1534;2)_0] \} \\ &\hspace{20em} (A-2) \end{aligned}$$

$$\begin{aligned} \bar{\Phi}_f\left(-\frac{1}{2}\right) &= \frac{N_f}{3!2!\sqrt{3}} (\alpha_3\beta_4 - \beta_3\alpha_4) \{ \sqrt{2} [(\alpha_1\beta_2 - \beta_1\alpha_2) \beta_5 (1234;5)_0 \\ &\quad - \beta_1 (\beta_2\alpha_5 - \alpha_2\beta_5) (5234;1)_0 - \beta_2 (\alpha_1\beta_5 - \beta_1\alpha_5) (1534;2)_0] \\ &\quad + [(\alpha_1\beta_2 - \beta_1\alpha_2) \alpha_5 (1234;5)_{-1} - \alpha_2 (\alpha_1\beta_5 - \beta_1\alpha_5) (1534;2)_{-1} \\ &\quad - \alpha_1 (\beta_2\alpha_5 - \alpha_2\beta_5) (5234;1)_{-1}] \} \\ &\hspace{20em} (A-3) \end{aligned}$$

$$\begin{aligned} \bar{\Phi}_f\left(-\frac{3}{2}\right) &= \frac{N_f}{3!2!} (\alpha_3\beta_4 - \beta_3\alpha_4) [(\alpha_1\beta_2 - \beta_1\alpha_2) \beta_5 (1234;5)_{-1} \\ &\quad - \beta_1 (\beta_2\alpha_5 - \alpha_2\beta_5) (5234;1)_{-1} - \beta_2 (\alpha_1\beta_5 - \beta_1\alpha_5) (1534;2)_{-1}] \\ &\hspace{20em} (A-4) \end{aligned}$$

The number in the parenthesis on the left hand side of each equation denotes the magnetic quantum number M_J .

N_f is a normalization constant , which can be determined from the equation

$$\langle \bar{\Phi}_f | \bar{\Phi}_f \rangle = 1 = \langle \varphi_f | \bar{\Phi}_f \rangle$$

where φ_f is the unantisymmetrized wave function.

APPENDIX B

1. Coefficients of the Quadratic

Polynomial of the Exponential in $(5234;1)_m^*$

$$\begin{aligned} \phi_1 = & A_1 R^2 + B_1 \bar{r}_2^2 + C_1 \bar{r}_3^2 + D_1 \bar{r}_4^2 + E_1 R_{cm}^2 + F_1 R \cdot \bar{r}_2 + G_1 R \cdot \bar{r}_3 \\ & + H_1 R \cdot \bar{r}_4 + I_1 \bar{r}_2 \cdot \bar{r}_3 + J_1 \bar{r}_2 \cdot \bar{r}_4 + K_1 \bar{r}_3 \cdot \bar{r}_4 \end{aligned}$$

Coefficients	Dependence on parameters	Numerical values (10^{25} cm^{-2})
A_1	$\frac{12}{25} \alpha_1 + \frac{9}{10} \beta'$	4.1034
		5.0034
B_1	$\frac{3}{8} \alpha_1 + \frac{5}{8} \beta'$	3.030
		3.655
C_1	$\frac{3}{8} \alpha_1 + \frac{5}{8} \beta'$	3.030
		3.655
D_1	α_1	4.33
F_1	$\frac{3}{10} \alpha_1 - \frac{3}{2} \beta'$	-2.076
		-3.576
G_1	$\frac{3}{10} \alpha_1 - \frac{3}{2} \beta'$	-2.076
		-3.576
H_1	$\frac{6}{5} \alpha_1$	5.196
I_1	$-\frac{1}{4} \alpha_1 + \frac{5}{4} \beta'$	1.73
		2.98
J_1	no dependence	0
K_1	no dependence	0

2. Coefficients of the Quadratic
Polynomial of the Exponential in (123;45)

$$\Phi_2 = A_2 R^2 + B_2 \bar{r}_2^2 + C_2 \bar{r}_3^2 + D_2 \bar{r}_4^2 + E_2 R_{cm}^2 + F_2 R \cdot \bar{r}_2 + G_2 R \cdot \bar{r}_3$$

$$+ H_2 R \cdot \bar{r}_4 + I_2 \bar{r}_2 \cdot \bar{r}_3 + J_2 \bar{r}_2 \cdot \bar{r}_4 + K_2 \bar{r}_3 \cdot \bar{r}_4$$

Coefficient	Dependence on parameters	Numerical value (10^{25} cm^{-2})
A_2	$\frac{12}{15} \alpha + \frac{9}{25} \bar{\alpha} + \frac{3}{5} \beta$	3.3228
B_2	α	2.81
C_2	α	2.81
D_2	$\bar{\alpha}$	4.78
F_2	$-\frac{6}{5} \alpha$	-3.372
G_2	$-\frac{6}{5} \alpha$	-3.372
H_2	$\frac{6}{5} \bar{\alpha}$	5.736
I_2	α	2.81
J_2	no dependence	0
K_2	no dependence	0

3. Coefficients of the Quadratic

Polynomial of the Exponential in (1234;5)_m*

$$\begin{aligned} \phi_1^i = & A_1^i R^2 + B_1^i \bar{r}_2^2 + C_1^i \bar{r}_3^2 + D_1^i \bar{r}_4^2 + E_1^i R_{cm}^2 + F_1^i R \cdot \bar{r}_2 \\ & + G_1^i R \cdot \bar{r}_3 + H_1^i R \cdot \bar{r}_4 + I_1^i \bar{r}_2 \cdot \bar{r}_3 + J_1^i \bar{r}_2 \cdot \bar{r}_4 + K_1^i \bar{r}_3 \cdot \bar{r}_4 \end{aligned}$$

Coefficient	Dependence on parameters	Numerical value (10 ²⁵ cm ⁻²)
A ₁ ⁱ	$\frac{27}{30} \alpha_1 + \frac{9}{10} \beta'$	4.3632 5.2632
B ₁ ⁱ	α_1	4.33
C ₁ ⁱ	α_1	4.33
D ₁ ⁱ	$\frac{3}{8} \alpha_1 + \frac{5}{8} \beta'$	3.03 3.655
F ₁ ⁱ	$-\frac{6}{5} \alpha_1$	-5.196
G ₁ ⁱ	$-\frac{6}{5} \alpha_1$	-5.196
H ₁ ⁱ	$-\frac{3}{10} \alpha_1 + \frac{3}{2} \beta'$	2.076 3.567
I ₁ ⁱ	α_1	4.33
J ₁ ⁱ	$-\frac{1}{4} \alpha_1$	-1.0825
K ₁ ⁱ	$\frac{1}{4} \alpha_1$	1.0825

APPENDIX C

Reduction of a Polynomial of
Quadratic Form to Diagonal Form (14)

Let the quadratic polynomial be

$$P = Ar_1^2 + Br_2^2 + Cr_3^2 + Dr_4^2 + Fr_1r_2 + Gr_1r_3 + Hr_1r_4 + Ir_2r_3 \\ + Jr_2r_4 + Kr_3r_4$$

In P, terms involving r_2 are

$$Br_2^2 + Fr_1r_2 + Ir_2r_3 + Jr_2r_4 \\ = B \left(r_2 + \frac{F}{2B} r_1 + \frac{I}{2B} r_3 + \frac{J}{2B} r_4 \right)^2 - \frac{1}{4B} (Fr_1 + Ir_3 + Jr_4)^2$$

Using the transformation

$$X_1 = r_1$$

$$X_2 = r_2 + \frac{F}{2B} r_1 + \frac{I}{2B} r_3 + \frac{J}{2B} r_4$$

(C-1)

$$X_3 = r_3$$

$$X_4 = r_4$$

P becomes

$$P = AX_1^2 + BX_2^2 + CX_3^2 + DX_4^2 + GX_1X_3 + HX_1X_4 + KX_3X_4 \\ - \frac{1}{4B} (FX_1 + IX_3 + JX_4)^2$$

$$= C_0 X_3^2 + G' X_1 X_3 + K' X_3 X_4 + \left(A - \frac{F^2}{4B}\right) X_1 + B X_2^2 + \left(D - \frac{J^2}{4B}\right) X_4^2 \\ + \left(H - \frac{FI}{2B}\right) X_1 X_4$$

where $C_0 = C - \frac{I^2}{4B}$

$$G' = G - \frac{FI}{2B}$$

$$K' = K - \frac{JI}{2B}$$

Rearranging terms in P, we have

$$P = C_0 \left(X_3 + \frac{G' X_1}{2C_0} + \frac{K' X_4}{2C_0}\right)^2 - \frac{1}{4C_0} (G' X_1 + K' X_4)^2 \\ + \left(A - \frac{F^2}{4B}\right) X_1^2 + B X_2^2 + \left(D - \frac{J^2}{4B}\right) X_4^2 + \left(H - \frac{FI}{2B}\right) X_1 X_4$$

Using the transformation

$$Y_1 = X_1$$

$$Y_2 = X_2$$

$$Y_3 = X_3 + \frac{G'}{2C_0} X_1 + \frac{K'}{2C_0} X_4$$

$$Y_4 = X_4$$

the only remaining cross product term is $Y_1 Y_4$:

$$P = C_0 Y_3^2 - \frac{1}{4C_0} (G' Y_1 + K' Y_4)^2 + \left(A - \frac{F^2}{4B}\right) Y_1 + B Y_2^2 \\ + \left(D - \frac{J^2}{4B}\right) Y_4 + \left(H - \frac{FI}{2B}\right) Y_1 Y_4$$

$$= A'Y_1 + BY_2 + C_0Y_3 + D_0Y_4 + H'Y_1Y_4$$

where $D_0 = D - \frac{J^2}{2E} - \frac{K'^2}{4C_0}$

$$H' = H - \frac{FJ}{2B} - \frac{G'K'}{2C_0}$$

$$A' = A - \frac{F^2}{4B} - \frac{G'^2}{4C_0}$$

To eliminate the term Y_1Y_4 , we use the same procedure as before.

$$\begin{aligned} P &= BY_2^2 + C_0Y_3^2 + D_0\left(Y_4 + \frac{H'}{2D_0}Y_1\right)^2 - \frac{1}{4D_0}(H'Y_1)^2 + A'Y_1^2 \\ &= \left(A' - \frac{H'^2}{4D_0}\right)Y_1^2 + BY_2^2 + C_0Y_3^2 + D_0\left(Y_4 + \frac{H'}{2D_0}Y_1\right)^2 \end{aligned}$$

Finally, using the transformation

$$\rho_1 = Y_1$$

$$\rho_2 = Y_2$$

$$\rho_3 = Y_3$$

$$\rho_4 = Y_4 + \frac{H'}{2D_0}Y_1$$

(C-3)

P is transformed into a diagonal form.

$$P = A_0\rho_1^2 + B\rho_2^2 + C_0\rho_3^2 + D_0\rho_4^2$$

where $C_0 = C - \frac{I^2}{4B}$

$$D_0 = D - \frac{J^2}{2B} - \frac{(K - \frac{JI}{2B})^2}{4C_0}$$

$$A_0 = A' - \frac{H'}{4D_0}$$

$$= A - \frac{F^2}{4B} - \frac{(G - \frac{FI}{2B})^2}{4C_0} - \frac{1}{4D_0} \left[H - \frac{FJ}{2B} - \frac{1}{2C_0} (G - \frac{FI}{2B})(K - \frac{JI}{2B}) \right]^2$$

Combining the three transformations in eqs.(C-1), (C-2) and (C-3), the total transformation is

$$\rho_1 = r_1$$

$$\rho_2 = r_2 + \frac{F}{2B} r_1 + \frac{I}{2B} r_3 + \frac{J}{2B} r_4$$

$$\rho_3 = \frac{G'}{2C'} r_1 + r_3 + \frac{K'}{2C'} r_4$$

$$\rho_4 = \frac{H'}{2D'} r_1 + r_4$$

(C-4)

The Jacobian of this transformation is

$$J = \frac{\partial (r_1, r_2, r_3, r_4)}{\partial (\rho_1, \rho_2, \rho_3, \rho_4)} = 1$$

The transformation inverse to (C-4) is

$$r_1 = \rho_1$$

$$r_2 = a_{21} \rho_1 + \rho_2 + a_{23} \rho_3 + a_{24} \rho_4$$

$$r_3 = a_{31} \rho_1 + \rho_3 + a_{34} \rho_4$$

$$r_4 = a_{41} \rho_1 + \rho_4$$

where

$$a_{41} = - \frac{H'}{2D_0}$$

$$a_{31} = \frac{K'H'}{4C_0D_0} - \frac{G'}{2C_0}$$

$$a_{34} = \frac{K'}{2C_0}$$

$$a_{21} = \frac{I}{2B} a_{31} - \frac{F}{2B} + \frac{J}{2B} a_{41}$$

$$a_{23} = \frac{I}{2B}$$

$$a_{24} = \frac{I}{2B} a_{34} + \frac{J}{2B}$$

(C-5)

APPENDIX D

Numerical Values of Constants in the Integrals L_{1m} and L_{2m}

L_{1m}		L_{2m}	
A_0	$\left. \begin{matrix} 2.316 \\ 2.467 \end{matrix} \right\} \times 10^{25} \text{ cm}^{-2}$	A'_0	$\left. \begin{matrix} 2.263 \\ 2.538 \end{matrix} \right\} \times 10^{25} \text{ cm}^{-2}$
B	$\left. \begin{matrix} 5.840 \\ 6.465 \end{matrix} \right\} \times 10^{25} \text{ cm}^{-2}$	B'	$7.140 \times 10^{25} \text{ cm}^{-2}$
C_0	$\left. \begin{matrix} 4.957 \\ 5.168 \end{matrix} \right\} \times 10^{25} \text{ cm}^{-2}$	C'_0	$5.355 \times 10^{25} \text{ cm}^{-2}$
D_0	$9.110 \times 10^{25} \text{ cm}^{-2}$	D'_0	$\left. \begin{matrix} 7.643 \\ 8.273 \end{matrix} \right\} \times 10^{25} \text{ cm}^{-2}$
e_1	$\begin{matrix} -2.641 \\ -2.288 \end{matrix}$	e'_1	$\begin{matrix} 3.445 \\ 3.186 \end{matrix}$
e_2	5.0		
e_3	$\begin{matrix} 3.056 \\ 2.761 \end{matrix}$		
e_4	0	e'_4	5.0
c_1	$\left. \begin{matrix} -0.264 \\ -0.165 \end{matrix} \right\} \times 10^{25} \text{ cm}^{-2}$	c'_1	$\left. \begin{matrix} 0.559 \\ 0.333 \end{matrix} \right\} \times 10^{25} \text{ cm}^{-2}$
c_2	0		
c_3	$2.81 \times 10^{25} \text{ cm}^{-2}$		
c_4	$4.78 \times 10^{25} \text{ cm}^{-2}$	c'_4	$4.354 \times 10^{25} \text{ cm}^{-2}$

APPENDIX E

1. Evaluation of $S_1^{(n)}(ij)$

$S_1^{(n)}(ij)$ is an integral of the form

$$S_1^{(n)}(ij) = \int e^{-\lambda r_{ij}^2} (x_i + iy_i - x_j - iy_j) (n)_1^* (123;45) d\tau$$

with $n = 1, 2, 3$, and $i, j = 1, 2, 3, 4, 5$.

$(n)_1$ stands for the final state wave function where $n = 1, 2, 3$ represent $(1234;5)_1$, $(5234;1)_1$ and $(1534;2)_1$ respectively.

Here only the method to evaluate $S_1^1(31)$ will be given in detail; all the others can be obtained in a similar way.

$$S_1^1(31) = \int e^{-\lambda r_{13}^2} (x_3 + iy_3 - x_1 - iy_1) (1234;5)_1^* (123;45) d\tau \quad (\text{E-1})$$

As in Chapter II, the coordinates can be transformed into a frame with \vec{R} , \vec{r}_2 , \vec{r}_3 , \vec{r}_4 and \vec{R}_{cm} as independent variables.

$$\begin{aligned} r_{13}^2 &= (\vec{r}_3 - \vec{r}_1)^2 \\ &= \left(-\frac{6}{5} \vec{R} + \vec{r}_2 + 2 \vec{r}_3 \right)^2 \\ &= \frac{36}{25} R^2 + r_2^2 + 4 r_3^2 - \frac{12}{5} \vec{R} \cdot \vec{r}_2 - \frac{24}{5} \vec{R} \cdot \vec{r}_3 + 4 \vec{r}_2 \cdot \vec{r}_3 \quad (\text{E-1a}) \end{aligned}$$

$$x_3 + iy_3 - x_1 - iy_1 = -\sqrt{\frac{8\pi}{3}} \left[-\frac{6}{5} R Y_1(\Omega) + r_2 Y_1(\omega_2) + 2 r_3 Y_1(\omega_3) \right] \quad (\text{E-2})$$

The transformed wave functions are given by eqs.(3-22) and (3-39) with $rY_1^{1*}(\omega)$ used in place of $\sqrt{\frac{3}{4\pi}} z$.

In the new coordinate system, $S_1^{(1)}(31)$ becomes

$$S_1^{(1)}(31) = -\sqrt{\frac{8\pi}{3}} |J_1|^3 \frac{1}{4} \int \left[6RY_1^{1*}(\Omega) + 5\bar{r}_4 Y_1^{1*}(\omega_4) \right] \left[-RY^1(\Omega) + \bar{r} Y^1(\omega_2) + 2\bar{r} Y^1(\omega_3) \right] R^2 \exp\left[-(A''R^2 + B''\bar{r}_2^2 + C''\bar{r}_3^2 + D''\bar{r}_4^2 + E''R_{cm}^2 + F''\vec{R} \cdot \vec{r}_2 + G''\vec{R} \cdot \vec{r}_3 + H''\vec{R} \cdot \vec{r}_4 + I''\vec{r}_2 \cdot \vec{r}_3 + J''\vec{r}_2 \cdot \vec{r}_4 + K''\vec{r}_3 \cdot \vec{r}_4)\right] d\tau \quad (E-3)$$

where the exponential term is equal to the product of $e^{-\lambda r_{13}^2}$ and the exponential terms $(1234;5)_1^*(123;45)$. Thus, by eq.(E-1a)

$$A'' = A' + \frac{36}{25} \lambda$$

$$B'' = B' + \lambda$$

$$C'' = C' + 4 \lambda$$

$$D'' = D'$$

$$F'' = F' - \frac{12}{5} \lambda$$

$$G'' = G' - \frac{25}{4} \lambda$$

$$H'' = H'$$

$$I'' = I' + 4 \lambda$$

$$J'' = J'$$

$$K'' = K'$$

(E-4)

where A', B', C',, K' are the constants in eq.(3-41).

Using eqs.(3-30), eq.(E-3) is transformed to a new coordinate system such that all cross product terms in the exponential vanish. The product of r and the spherical harmonic function $Y_1^1(\omega)$ can be transformed as an ordinary coordinate in a quadratic form. To see this, we write $rY_1^1(\omega)$

as

$$rY_1^1(\omega) = -\sqrt{\frac{3}{8\pi}} \zeta = -\sqrt{\frac{3}{8\pi}} (x + iy)$$

$$rY_1^{1*}(\omega) = -\sqrt{\frac{3}{8\pi}} \zeta^* = -\sqrt{\frac{3}{8\pi}} (x - iy)$$

(E-5)

The product of two linear combinations of $rY_1^1(\omega)$ can be written in the form

$$d_{11} \zeta_1^* \zeta_1 + d_{22} \zeta_2^* \zeta_2 + \dots + d_{44} \zeta_4^* \zeta_4 + d_{12} \zeta_1^* \zeta_2$$

$$+ d_{13} \zeta_1^* \zeta_3 + \dots + d_{34} \zeta_3^* \zeta_4$$

This can be transformed to another quadratic form by a transformation; the coefficients of the transformed quadratic form are given by the matrix equation

$$C = \tilde{T} D T \tag{E-6}$$

where D and C are the matrices corresponding to the coefficients of the original and the transformed quadratic form, and T and \tilde{T} are the transformation matrix and its transpose. Then, using eqs.(E-5), the new quadratic form can be written in terms of the new coordinates $\rho_1, \rho_2, \rho_3, \rho_4$ and the corresponding spherical harmonics.

$S_1^{(1)}(31)$ is transformed into new coordinate system \vec{P}_1 , \vec{P}_2 , \vec{P}_3 , \vec{P}_4 by eqs.(3-30).

$$\begin{aligned}
 S_1^{(1)}(31) = & -\frac{c^3}{4} \sqrt{\frac{8\pi}{3}} \int [c_{11} \rho_1^2 Y_1^{1*}(\Omega_1) Y_1^1(\Omega_1) + c_{22} \rho_2^2 Y_1^{1*}(\Omega_2) Y_1^1(\Omega_2) \\
 & + c_{33} \rho_3^2 Y_1^{1*}(\Omega_3) Y_1^1(\Omega_3) + c_{44} \rho_4^2 Y_1^{1*}(\Omega_4) Y_1^1(\Omega_4) \\
 & + c_{12} \rho_1 \rho_2 Y_1^{1*}(\Omega_1) Y_1^1(\Omega_2) + c_{13} \rho_1 \rho_3 Y_1^{1*}(\Omega_1) Y_1^1(\Omega_3) \\
 & + \dots + c_{34} \rho_3 \rho_4 Y_1^{1*}(\Omega_3) Y_1^1(\Omega_4)] \rho^2 \exp[-(A_0'' \rho_1^2 \\
 & + B'' \rho_2^2 + C_0'' \rho_3^2 + D_0'' \rho_4^2)] \rho_1^2 \rho_2^2 \rho_3^2 \rho_4^2 d\Omega_1 d\Omega_2 d\Omega_3 d\Omega_4
 \end{aligned}
 \tag{E-7}$$

where the c's are given by eq.(E-6).

Here the term corresponding to the motion of the centre of mass has been dropped for the same reason as it was in the calculation of L_{1m} (page 30). It is obvious from eq.(E-7) that all variables are separable and the integration can be carried out analytically term by term. The contributions from terms of the form $\rho_i \rho_j Y_1^{1*}(\Omega_i) Y_1^1(\Omega_j)$ ($i \neq j$) vanish due to the orthogonality of the spherical harmonics.

Then,

$$\begin{aligned}
 S_1^{(1)}(31) = & -\sqrt{\frac{8\pi}{3}} \frac{81\pi^5}{8} \frac{1}{A_0''(A_0''B''C_0''D_0'')^{3/2}} \left(\frac{5c_{11}}{A_0''} + \frac{3c_{22}}{B''} \right. \\
 & \left. + \frac{3c_{33}}{C_0''} + \frac{3c_{44}}{D_0''} \right)
 \end{aligned}
 \tag{E-8}$$

For the other $S_1^{(1)}(ij)$, eq.(E-8) is also valid. Only numerical changes of the values for the c's and A_0'' , B'' , C_0'' ,

D_0'' are needed.

The evaluation of $S_1^{(2)}(ij)$ differs from that of $S_1^{(1)}(ij)$ only in the wave function used; that is, $(5234;1)_1^*$ is substituted in place of $(1234;5)_1^*$. From eq.(3-19),

$$(5234;1)_1^* = \frac{1}{4} \left[-6RY_1^{1*}(\Omega) + 5\bar{r}_2 Y_1^{1*}(\omega_2) + 5\bar{r}_3 Y_1^{1*}(\omega_3) \right] \exp \left[-(A_1 \bar{r}_1^2 + B_1 \bar{r}_2^2 + C_1 \bar{r}_3^2 + D_1 \bar{r}_4^2 + \dots + K_1 \bar{r}_3 \cdot \bar{r}_4) \right]$$

Analogous to eq.(E-3), it can be shown that

$$S_1^{(2)}(31) = -\sqrt{\frac{8\pi}{3}} |J_1|^{-3} \frac{1}{4} \int \left[-6RY_1^{1*}(\Omega) + 5\bar{r}_2 Y_1^{1*}(\omega_2) + 5\bar{r}_3 Y_1^{1*}(\omega_3) \right] \left[-RY_1^1(\Omega) + \bar{r}_2 Y_1^1(\omega_2) + 2\bar{r}_3 Y_1^1(\omega_3) \right] R^2 \exp \left[-(A''R + B''\bar{r}_2^2 + \dots + K''\bar{r}_3 \cdot \bar{r}_4) \right] d\tau$$

The relations in eqs.(E-4) hold for this integral.

A', B', C', \dots, K' in eqs.(E-4) are now the coefficients of the exponential term in $(5234;1)_1^*(123;45)$.

The subsequent steps follow directly from eqs.(E-4) to (E-8); only the numerical values of the constants in eq.(E-8) are different. Expressions for $S_1^{(2)}(ij)$ for other i, j can be worked out in a similar way.

For the evaluation of $S_1^{(3)}(ij)$, since the wave function $(1534;2)_1^*$ has not been calculated previously, we have to first transform it to the new coordinate system. The result is

$$\begin{aligned}
 (1534;2)_1^* &= \exp\left(-\frac{\alpha'}{2} \sum_1 r_i'^2\right) R_1 Y_1^{1*}(\Omega_1) e^{-\frac{2\beta'}{5} R_1^2} e^{-\frac{5\gamma}{2} R_{cm}^2} \\
 &= \frac{1}{4} \left[-5\vec{r}_2 Y_1(\Omega_2)\right] \exp\left[-(A_0 R^2 + B_3 \vec{r}_2^2 + \dots + K_3 \vec{r}_3 \cdot \vec{r}_4)\right]
 \end{aligned}$$

where $\vec{r}_i'' = \vec{r}_i - \vec{R}_\alpha$ ($i = 1, 5, 3, 4$)

$$\vec{R}_\alpha = \frac{1}{4} (\vec{r}_1 + \vec{r}_5 + \vec{r}_3 + \vec{r}_4)$$

$$\vec{R}_1 = \vec{R}_\alpha - \vec{r}_2$$

The factor $\frac{1}{4}$ has been taken out in order to give it a form analogous to $(1534;2)_1^*$; the result is applicable without change of numerical factors. The form of $S_1^{(3)}(ij)$ is given by eq.(E-8).

2. Evaluation of $M_{-1}(x-iy)$, $N_{-1}(x-iy)$ and $N_0(z)$

To calculate $M_{-1}(x-iy)$, $N_{-1}(x-iy)$ and $N_0(z)$, it is only necessary to change a few things in the derivation for $N_1(x+iy)$ and $M_1(x+iy)$.

Let

$$N_{-1}(x-iy) = N_{-1}^{(1)} + N_{-1}^{(2)} + N_{-1}^{(3)}$$

$N_{-1}^{(1)}$ is given by eq.(4-26) with $x+iy-x-iy$ replaced by $x-iy-(x-iy)$. From eqs.(4-27) to (4-32), $S_1^{(n)}(ij)$ is replaced by $S_{-1}^{(n)}(ij)$. To evaluate $S_{-1}^{(n)}(ij)$, we follow the procedure from eq.(E-2) to eq.(E-8). Eq.(E-2) is changed to

$$x_3 - iy_3 - (x_1 - iy_1) = \sqrt{\frac{8\pi}{3}} \left[-\frac{6}{3} rY_1^{-1}(\Omega) + \bar{r}_2 Y_1^{-1}(\omega_2) + 2\bar{r}_3 Y_1^{-1}(\omega_3) \right]$$

By comparing this equation with eq.(E-2), it is seen that there is a change of sign for the m in Y_1^m and for the whole expression. Henceforth, the changes from eq.(E-2) to eq.(E-8) are the replacement of Y_1^{1*}, Y_1^1 by Y_1^{-1*}, Y_1^{-1} , and a change of sign for the whole expression. Because the m in the spherical harmonics does not enter eq.(E-8), we conclude that

$$N_{-1}(x-iy) = -N_1(x+iy)$$

$$M_{-1}(x-iy) = -M_1(x+iy)$$

Finally, for $N_0(z)$, $S_1^{(1)}(ij)$ is replaced by $S_0^{(1)}(ij)$ from eq.(4-27) to eq.(4-32), and instead of eq.(E-2), we have

$$z_3 - z_1 = \sqrt{\frac{4\pi}{3}} \left[-\frac{6}{3} rY_1^0(\Omega) + \bar{r}_2 Y_1^0(\omega_2) + 2\bar{r}_3 Y_1^0(\omega_3) \right]$$

Here both sign and numerical factor have been changed. In the subsequent steps, $-\sqrt{\frac{8\pi}{3}} rY_1^1$ is replaced by $\sqrt{\frac{4\pi}{3}} rY_1^0$. Therefore,

$$S_0^{(1)}(31) = -\frac{1}{\sqrt{2}} S_1^{(1)}(31)$$

and

$$N_0(z) = -\frac{1}{\sqrt{2}} N_1(x+iy)$$

APPENDIX F

Numerical Values of the Constants
in the Integrals $S_1^{(n)}(ij)$ and Values of $S_1^{(n)}(ij)$

In the following table, for each ${}^{(n)}_1(ij)$, the first two rows are values of A_0'' , B'' , C_0'' and D_0'' , corresponding to two different values of the parameters β' , λ and V_{LS} . The third and fourth rows are values of c_{11} , c_{22} , c_{33} , c_{44} and $S_1^{(n)}(ij)$.

${}^{(n)}_1(ij)$	$A_0'' (10^{25} \text{cm}^{-2})$	$B'' (10^{25} \text{cm}^{-2})$	$C_0'' (10^{25} \text{cm}^{-2})$	$D_0'' (10^{25} \text{cm}^{-2})$	$S_1^{(n)}(ij) (10^{19.8} \text{cm}^{16})$
	c_{11}	c_{22}	c_{33}	c_{44}	
${}^{(1)}_1(31)$	2.269	9.797	9.711	7.670	
	2.544	11.3	11.269	8.302	
	0.107	0	0	-0.304	-0.685
	0.081	0	0	-0.227	-0.196
${}^{(1)}_1(32)$	2.288	9.797	9.712	7.744	
	2.574	11.3	11.269	8.388	
	0.213	0	0	-0.609	-1.307
	0.163	0	0	-0.455	-0.371
${}^{(1)}_1(35)$	4.178	7.14	8.012	8.624	
	4.989	7.14	9.515	9.959	
	1.529	0	0	2.335	-6.457
	1.084	0	0	2.387	-1.654
${}^{(1)}_1(41)$	3.852	9.797	5.839	9.421	
	4.230	11.3	6.012	10.615	
	-2.082	0	0	3.341	4.031
	-1.794	0	0	2.814	1.667
${}^{(1)}_1(42)$	3.320	9.797	5.839	8.924	
	4.035	11.3	6.012	9.951	
	-1.980	0	0	2.835	7.853
	-1.666	0	0	2.387	2.098

$\binom{n}{1}(ij)$	$A_0'' (10^{25} \text{cm}^{-2})$	$B'' (10^{25} \text{cm}^{-2})$	$C_0'' (10^{25} \text{cm}^{-2})$	$D_0'' (10^{25} \text{cm}^{-2})$	$S_1^{(n)}(ij) (10^{19} \text{cm}^{-6})$
	c_{11}	c_{22}	c_{33}	c_{44}	
$\binom{1}{1}(45)$	2.298 2.546	7.14 7.14	5.355 5.355	18.273 24.913	
	0.237 0.075	0 0	0 0	10.0 10.0	-13.084 -3.988
$\binom{2}{1}(31)$	2.351 2.476	8.497 10.625	9.698 11.267	9.11 9.11	
	0.156 0.051	5.0 5.0	0.594 -0.262	0 0	-11.731 -3.729
$\binom{2}{1}(32)$	2.316 2.467	8.497 10.625	8.479 10.474	9.11 9.11	
	0 0	-5.0 -5.0	4.929 4.929	0 0	0 0
$\binom{2}{1}(35)$	3.590 4.193	5.84 6.465	7.614 9.328	10.839 11.414	
	-1.782 -1.436	0 0	3.056 2.761	-0.694 -0.682	5.100 1.383
$\binom{2}{1}(41)$	4.534 4.452	8.497 10.625	5.64 5.940	10.715 11.312	
	0.578 0.128	5.0 5.0	0.882 0.564	-1.195 -1.245	-4.468 -11.697
$\binom{2}{1}(42)$	3.590 4.202	8.497 10.625	5.233 5.676	10.839 11.414	
	1.782 1.392	-5.0 -5.0	0.978 0.991	0.694 0.682	-5.100 -1.299
$\binom{2}{1}(45)$	2.316 2.467	5.840 6.465	4.957 5.168	19.738 25.750	
	0 0	0 0	0 0	0 0	0 0
$\binom{3}{1}(31)$	2.576 2.610	8.497 10.125	8.479 9.817	9.11 9.11	
	0 0	-5.0 -5.0	4.989 4.848	0 0	0 0

${}^{(n)}_1(ij)$	$A''_0(10^{25} \text{cm}^2)$	$B''_0(10^{25} \text{cm}^2)$	$C''_0(10^{25} \text{cm}^2)$	$D''_0(10^{25} \text{cm}^2)$	$S''_1(ij)(10^{19} \text{cm}^6)$
	c_{11}	c_{22}	c_{33}	c_{44}	
${}^{(3)}_1(32)$	2.611	8.497	9.698	9.11	
	2.736	10.025	11.267	9.11	
${}^{(3)}_1(35)$	1.222	10.0	0.652	0	-24.034
	0.956	10.0	-0.246	0	-9.058
${}^{(3)}_1(35)$	3.849	5.84	7.614	10.839	
	4.462	6.465	9.328	11.414	
${}^{(3)}_1(41)$	-1.782	0	3.053	-0.694	3.795
	-1.392	0	2.761	-0.682	1.005
${}^{(3)}_1(41)$	3.849	8.497	5.233	10.839	
	4.229	10.125	5.398	11.381	
${}^{(3)}_1(42)$	1.782	-5.0	0.798	0.694	-3.795
	1.480	-5.0	0.903	0.741	-1.516
${}^{(3)}_1(42)$	4.423	8.497	5.64	7.559	
	4.207	10.125	5.881	4.969	
${}^{(3)}_1(45)$	-0.160	5.0	0.882	-0.824	-5.455
	-0.531	5.0	0.621	-0.012	-5.625
${}^{(3)}_1(45)$	2.576	5.840	4.957	19.738	
	2.618	6.465	5.168	25.450	
${}^{(3)}_1(45)$	0	0	0	0	0
	0.032	0	0	0	-0.201

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