CLUSTER MODEL CALCULATIONS ON THE LOWEST THREE STATES OF ^{5}He

by

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ABSTRACT

The cluster model wavefunction of the $3/2^-$ and $3/2^+$ state of ^{5}He are decomposed into a sum of shell model harmonic oscillator wavefunctions. About 97% of the $3/2^-$ state was accounted for, whereas only 6% of the $3/2^+$ state was found. An attempt to determine a cluster model wavefunction for the $1/2^-$ state of ^{5}He by fitting the experimentally measured values for the excitation energy and radiative width was unsuccessful.

A method for evaluating the integrals involved is introduced which could be of significant use in other similar calculations.

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CHAPTER 1

INTRODUCTION

In the past (1,2,3), much work has been done on the ^{5}He nucleus using the cluster model approach. Can there be any further justification for still further work on this particular nucleus? It is the author's belief that more can be learned about ^{5}He from this basic approach. The purpose of this thesis is to report two further attempts at gaining insight into the structure of this nucleus.

The first problem to be discussed is not new; it was originally attempted by Lee (3). The motivation for doing this problem again is that the previous calculation was found to be in error. This was found when an attempt was made to extend the calculation and it proved to be impossible to reproduce Lee's results. Consequently, the entire calculation has been redone.

Very rarely is a nuclear state described completely by a pure shell model wavefunction. It is often the practice in such calculations to represent a nuclear state by an admixture of pure shell model wavefunctions. This is possible because these wavefunctions form a complete set. The objective of such a procedure is to obtain a more realistic wavefunction of the given state. What has been attempted here is the exact reverse of this; that is, beginning with cluster model wavefunctions which represent the ground and second excited states of ^{5}He, the contributions of shell model configurations to these cluster model wavefunctions are calculated. This is accomplished by calculating the square of the overlap integral between the cluster model wavefunction and the appropriate shell model wavefunctions. Since the cluster model provides very good descriptions of certain properties of ^{5}He (1,4), it is of interest to know which shell model configurations are contained in a particular cluster model wavefunction. This information will provide a link between the cluster model and the more extensively used shell model.

In subsequent chapters the method used to perform this calculation will be outlined. To the author's knowledge this approach has not been used in this connection before, and in any case, it is thought that it could be quite useful in more involved calculations.

Pearlstein et. al.(4) were able to find a consistent set of width parameters for the cluster model wavefunction for the ground state and the second excited state of ^{5}He by doing a variational calculation on the energy of these states. They were unable, however, to find a set of width parameters for the first excited state which minimized the energy. In an attempt to find a set of cluster model parameters, we have tried to fit simultaneously the experimental data on the energy and the radiative width of this state.

The reason for renewed interest in this state is the recent publication of some new measurements related to ^{5}He. Buss et. al. (5) have measured the ratio of the radiative transition probability from the second excited state to the ground state to the radiative transition probability from the second excited state to the first state. Thus data is now available on a second parameter associated with this state, in addition to its excitation energy. The energy and radiative width of this state were calculated as functions of the width parameters in order to ascertain if a consistent set of parameters could be found to describe this particular state.

Chapter 2 will be concerned with the formalism for decomposing the ground state cluster model wavefunction into shell model wavefunctions. The second excited state will be dealt with similarly in Chapter 3. Chapter 4 will contain the results of the computations involved in these calculations and a discussion of their significance. Chapter 5 will present the formalism for the attempt to determine a set of width parameters to fit the data on the first excited state; discussion of this problem will follow in Chapter 6.

CHAPTER 2

DECOMPOSITION OF THE GROUND STATE CLUSTER MODEL WAVEFUNCTION

2.1 INTRODUCTION

This chapter will be concerned with the derivation of the formalism required to decompose the cluster model wavefunction of the ground $(3/2^-)$ state of ^{5}He into a sum of harmonic oscillator shell model wavefunctions. The cluster model wavefunction was proposed first by Pearlstein et. al. (4). Explicitly it is given by the expression

$$\Phi(\tfrac{3}{2}^-) = \exp\left(-\tfrac{1}{2}\alpha' \sum_{i}^{1,4} r'^{\,2}_i\right) R_1 Y_1^m(\Omega_1) \exp\left(-\tfrac{2}{5}\beta' R_1^{\,2}\right) \exp\left(-\tfrac{5}{2}\mu R_{cm}^{\,2}\right) \qquad \ldots(2\text{-}1)$$

where

$$\bar{r}_i' = \bar{r}_i - \frac{1}{4}\sum_{j}^{1,4} \bar{r}_j$$

$$\bar{R}_1 = \frac{1}{4}\sum_{j}^{1,4} \bar{r}_j - \bar{r}_5$$

$$\bar{R}_{cm} = \frac{1}{5}\sum_{j}^{1,5} \bar{r}_j$$

This wavefunction will be written as (1234;5), in a notation used by many authors (1,6).

The wavefunction appearing in eq. (2-1) is a product of three wavefunctions; the first represents the internal state of the alpha-particle cluster, the second represents the relative motion between the alpha-particle cluster and the neutron, and the third represents the motion of the centre-of-mass of the nucleus relative to some fixed spatial point. In previous calculations using this wavefunction (1,2,4), the value of the width parameter of the centre-of-mass motion was not of particular importance. The centre-of-mass motion of the nucleus could always be split off from the internal motion in the cluster model wavefunction; consequently, no spurious states arise. This means that only four coordinates are essentially involved instead of five; arbitrariness of the centre-of-mass width parameter is unimportant as long as only cluster model wavefunctions are being considered. Since the shell model wavefunctions are given in single-particle coordinates, it would be extremely difficult to split off the centre-of-mass motion. In order that the present calculations be independent of this motion, the value of the width parameter for the centre-of-mass motion has been chosen to be the same as that of the shell model wavefunctions.

The harmonic oscillator shell model wavefunctions are direct products of five single-particle wavefunctions.

There are two basic restrictions governing the selection of shell model configurations: the single-particle states must couple together to give the correct total angular momentum, and they must have the same parity as the cluster model wavefunction. After these two criteria have been satisfied, the selection is guided by the physics of the problem. First, those configurations describing lower energy states are likely to be most important. Second, configurations in which the occupancy of levels in the shell model reflects cluster configurations in the cluster model will be more important. The notation for these shell model wavefunctions will be $(12345)_i$, where the i is the indicator for the particular configuration.

Since the antisymmetrization operator is a projector, only one of the wavefunctions involved in an integral need by antisymmetrized. The cluster model wavefunction has been chosen to be antisymmetrized. Therefore, the same representation of any shell model configuration can be used in both the direct and exchange integrals.

The complete cluster model wavefunction of the $3/2^-$ state may be written symbolically before antisymmetrization as (1)

$$\Phi_{CM} = N_{CM} \,(1234;5)\, \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \qquad (2\text{-}2)$$

The antisymmetrized cluster model wavefunction is

$$A\Phi_{CM} = \frac{N_{CM}}{12} (\alpha_3\beta_4 - \beta_3\alpha_4) \{(\alpha_1\beta_2 - \beta_1\alpha_2)\alpha_5 \; (1234;5)$$
$$- (\beta_2\alpha_5 - \alpha_2\beta_5)\alpha_1 \; (5234;1) + (\beta_1\alpha_5 - \alpha_1\beta_5)\alpha_2 (1534;2)\} \quad ..(2\text{-}3)$$

The complete shell model wavefunctions before antisymmetrization have the same form as eq. (2-2), except for the change in notation for the spatial part (3). The same is true of the antisymmetrized shell model wavefunctions and eq. (2-3).

The details of the analysis for the calculation of the normalization constants are given in Appendix A.

2.2 THE EXPANSION COEFFICIENT

Any square-integrable wavefunction can be approximated as a convergent series of orthonormal functions, each of which is weighted by its own expansion coefficient (7). The expansion coefficient in the present case is the overlap integral between the cluster model wavefunction and the appropriate shell model wavefunction, both normalized to unity. Since the expansion coefficients satisfy the Parseval relation, it follows that if enough shell model configurations are considered then the sum of the squares of their expansion coefficients will equal 100%, due to the completeness of the set of shell model wavefunctions.

The expressions for the expansion coefficient for the ground state of ^{5}He have been written by Lee (3); they are given by

$$
\begin{aligned}
a_i &= \langle \Phi_{SM_i} | \, A\Phi_{CM} \rangle \\
&= \frac{N_{SM_i} \, N_{CM}}{12} \{ \langle (12345)_i | \, (1234;5) - (5234;1) \rangle \}
\end{aligned}
\qquad ..(2\text{-}4)
$$

where N_{SM_i} and N_{CM} are the normalization constants for the shell model and cluster model wavefunctions respectively.

2.3 THE OVERLAP INTEGRAL

i) The first five-particle configuration to be considered will be $(1s)^4(1p)$. This is the lowest energy shell model configuration appropriate to this state. Furthermore, if all the cluster model width parameters are put equal to the shell model width parameter, the antisymmetrized cluster model wavefunction is equivalent to this configuration, as shown by Lee (3).

This state may be represented by

$$(12345)_1 = \exp\left(-\frac{1}{2}\mu \sum_{i}^{1,5} r_i^{\,2}\right) r_5 \, Y_1^m(\Omega_5) \qquad (2\text{-}5)$$

where $Y_1^m(\Omega_5)$ is a spherical harmonic of order 1, and the arguments are the angular coordinates of the fifth nucleon.

In a single-particle representation, the direct integral appearing in eq. (2-4) is

$$\langle (12345)_1 | (1234;5) \rangle = \int \exp(-\varphi_1) r_5 Y_1^{m*}(\Omega_5) \left[\frac{1}{4} r_1 Y_1^m(\Omega_1) + \frac{1}{4} r_2 Y_1^m(\Omega_2) + \frac{1}{4} r_3 Y_1^m(\Omega_3) + \frac{1}{4} r_4 Y_1^m(\Omega_4) - r_5 Y_1^m(\Omega_5)\right] d\bar{r}_1 \, d\bar{r}_2 \, d\bar{r}_3 \, d\bar{r}_4 \, d\bar{r}_5 \qquad (2\text{-}6)$$

where $\varphi_1 = V(r_1^{\,2} + r_2^{\,2} + r_3^{\,2} + r_4^{\,2}) + W r_5^{\,2}$

$+ X(\bar{r}_1 . \bar{r}_2 + \bar{r}_1 . \bar{r}_3 + \bar{r}_1 . \bar{r}_4 + \bar{r}_2 . \bar{r}_3 + \bar{r}_2 . \bar{r}_4 + \bar{r}_3 . \bar{r}_4)$

$+ Z(\bar{r}_1 . \bar{r}_5 + \bar{r}_2 . \bar{r}_5 + \bar{r}_3 . \bar{r}_5 + \bar{r}_4 . \bar{r}_5)$

$$V = \frac{3}{5}\mu + \frac{3}{8}\alpha' + \frac{1}{40}\beta'$$

$$W = \frac{3}{5}\mu + \frac{2}{5}\beta'$$

$$X = -\frac{1}{4}\alpha' + \frac{1}{20}\beta' + \frac{1}{5}\mu$$

$$Z = \frac{1}{5}(\mu - \beta')$$

The single-particle representation of the exchange integral which appears in eq. (2-4) is

$$\langle (12345)_1 | (5234;1) \rangle = \int \exp(-\varphi_2) r_5 Y_1^{m*}(\Omega_5) [-r_1 Y_1^m(\Omega_1) + \frac{1}{4} r_2 Y_1^m(\Omega_2) + \frac{1}{4} r_3 Y_1^m(\Omega_3) + \frac{1}{4} r_4 Y_1^m(\Omega_4) + \frac{1}{4} r_5 Y_1^m(\Omega_5)] d\bar{r}_1 \, d\bar{r}_2 \, d\bar{r}_3 \, d\bar{r}_4 \, d\bar{r}_5 \qquad (2\text{-}7)$$

where

$$\varphi_2 = W r_1^2 + V(r_2^2 + r_3^2 + r_4^2 + r_5^2) + X(\bar{r}_2 . \bar{r}_3 + \bar{r}_2 . \bar{r}_4 + \bar{r}_2 . \bar{r}_5 + \bar{r}_3 . \bar{r}_4 + \bar{r}_3 . \bar{r}_5 + \bar{r}_4 . \bar{r}_5) + Z(\bar{r}_1 . \bar{r}_2 + \bar{r}_1 . \bar{r}_3 + \bar{r}_1 . \bar{r}_4 + \bar{r}_1 . \bar{r}_5)$$

The shell model normalization constant for this configuration is given in Table 4. The details of the procedure for evaluating these integrals appear in Appendix B. The method used allows them to be expressed in a closed form; furthermore, they both assume the same form. Thus for this particular shell model configuration the integrals reduce to the form

$$\frac{24\Pi^{13/2} E(2)}{E(1) [E(1) E(3) E(6) E(10) E(15)]^{3/2}} \qquad (2\text{-}8)$$

where the E's are coefficients which are obtained in the diagonalization of the quadratic form φ_1 and φ_2, and are defined in Appendix C.

Once the integrals are in this form, it is a relatively simple matter to compute the value of the expansion coefficient for any set of values of the width parameters. The discussion of this phase of the work will be deferred until Chapter 4.

ii) The next configuration to be considered is $(1s)^3(1p)(2s)$. Implicit in the cluster model wavefunction is a correlation between four nucleons. In the configuration considered in i), four of the nucleons are in the 1s shell, and so are strongly correlated by the Pauli principle; in the configuration presently under consideration, one of these four nucleons is in a 2s state. Thus the size of the coefficient of this configuration will indicate the strength of this correlation between the nucleons. If the coefficient is small, then it follows that four nucleons are strongly correlated in the cluster model wavefunction.

This state may be represented by

$$(12345)_2 = \exp\left(-\frac{1}{2}\mu \sum_{i}^{1,5} r_i^{\,2}\right) r_5 Y_1^m(\Omega_5)\left[\frac{3}{2} - \mu r_2^{\,2}\right] \qquad (2\text{-}9)$$

Table 4 contains the algebraic expression for the normalization constant for this configuration. Appendix B contains the details of the evaluation of the integral of the product of this wavefunction and the cluster model wavefunction. As in the first configuration considered, the direct and exchange integrals can both be expressed in the same form. In this case, it is

$$\frac{12\pi^{13/2}}{[E(1)\ E(3)\ E(6)\ E(10)\ E(15)]^{3/2}}\left[\frac{E(2)\ E(4)}{E(1)}\left\{3-\frac{5\mu}{E(1)}\right\}+\frac{3E(5)}{E(3)}\left\{1-\frac{\mu}{E(1)}\right\}\right] \qquad (2\text{-}10)$$

iii) The next state to be considered is $(1s)^4(2p)$. This describes the situation in which the neutron outside the 1s state is in the next highest shell consistent with parity and angular momentum considerations. This configuration may be represented by

$$(12345)_3 = \exp\left(-\tfrac{1}{2}\mu\sum_{i}^{1,5} r_i^{\,2}\right)\left(\tfrac{5}{2}-\mu r_5^{\,2}\right)r_5 Y_1^m(\Omega_5) \qquad (2\text{-}11)$$

The expression for the normalization constant is again found in Table 4, and the details for evaluating the overlap integrals are given in Appendix B. The closed form for these integrals is

$$\frac{60\pi^{13/2}}{E(1)\ [E(1)\ E(3)\ E(6)\ E(10)\ E(15)]^{3/2}}\left[1-\frac{\mu}{E(1)}\right] \qquad ..(2\text{-}12)$$

iv) The next state to be considered is $(1s)^4(3p)$. This describes a situation similar to that of the previous configuration, but with the extra nucleon in still the next higher shell consistent with parity and angular momentum considerations. This state may be represented by

$$(12345)_4 = \exp\left(-\frac{1}{2}\mu \sum_{i}^{1,5} r_i^2\right) \left(\frac{35}{8} - \frac{7}{2}\mu\, r_5^2 + \frac{1}{2}\mu^2 r_5^4\right) r_5 Y_1^m(\Omega_5) \qquad ..(2\text{-}13)$$

As in the previous cases, the details of the calculations are found in Appendices A and B. The closed form for the integrals in this case is

$$\frac{210\pi^{13/2}\, E(2)}{E(1)\,[E(1)\; E(3)\; E(6)\; E(10)\; E(15)]^{3/2}} \left[\frac{1}{2} - \frac{\mu}{E(1)} + \frac{1}{2}\left(\frac{\mu}{E(1)}\right)^2\right] \qquad (2\text{-}14)$$

The discussion of the numerical results appears in Chapter 4.

v) The coefficients for the configurations $(1s)^2(1p)^3$, $(1s)^2(1p)(2s)^2$ and $(1s)^3(1p)(3s)$ were calculated, but their contributions were each smaller than 0.001%. Although these states are low in energy, their shell structure does not reflect the cluster configuration assumed in the cluster model.

Specifically, the $(1s)^2(1p)^3$ configuration represents the situation in which two of the nucleons in the 1s level are promoted to the 1p level. The spatial wavefunction of this configuration is

$$(12345)_5 = \exp(-\tfrac{1}{2}\mu \sum_i^{1,5} r_i{}^2)\ r_2 r_3 r_5 |11\rangle_{523} \qquad (2\text{-}15)$$

where $|11\rangle_{523} = \frac{1}{2}[\,|11\rangle_5\,|1-1\rangle_2\,|11\rangle_3 - |1-1\rangle_5\,|11\rangle_2\,|11\rangle_3$

$\qquad + |11\rangle_5\,|10\rangle_2\,|10\rangle_3 - |10\rangle_5\,|11\rangle_2\,|10\rangle_3]$

The $(1s)^2(1p)(2s)^2$ configuration is similar to that of ii) except in this case a second nucleon is promoted from the 1s to the 2s level. This configuration may be represented by

$$(12345)_6 = \exp(-\tfrac{1}{2}\mu \sum_i^{1,5} r_i{}^2)\ (\tfrac{3}{2} - \mu_1 r_2{}^2)(\tfrac{3}{2} - \mu r_3{}^2)\ r_5 Y_1^m(\Omega_5) \qquad ..(2\text{-}16)$$

The $(1s)^3(1p)(3s)$ configuration is similar to that considered in section ii) except that one of the 1s nucleons is promoted to the 3s level instead of the 2s level. The spatial representation of this configuration is

$$(12345)_7 = \exp(-\tfrac{1}{2}\mu \sum_i^{1,5} r_i{}^2)\ [\tfrac{15}{8} - \mu r_2{}^2 + \tfrac{1}{2}\mu^2 r_2{}^4] r_5 Y_1^m(\Omega_5) \qquad ..(2\text{-}17)$$

Thus these configurations reflect the correlation intrinsic in the cluster model representation even less than that considered in ii). Therefore, it is not surprising that their contributions are small.

CHAPTER 3

DECOMPOSITION OF THE SECOND EXCITED STATE CLUSTER MODEL WAVEFUNCTION

3.1 INTRODUCTION

The purpose of this chapter is similar to that of the previous chapter except that here the second excited state will be considered. The wavefunction for this state was introduced in 1960 by Pearlstein et. al. along with that of the ground state (4). It has the form

$$\Phi(\tfrac{3}{2}^+) = \exp(-\tfrac{1}{2}\alpha \sum_{i}^{1,3} r_i''^2) \exp(-\tfrac{1}{2}\bar{\alpha} \sum_{j}^{4,5} r_j''^2) R^2$$

$$\exp(-\tfrac{3}{5}\beta R^2) \exp(-\tfrac{5}{2}\mu R^2_{cm}) \qquad (3\text{-}1)$$

where
$$\bar{r}_i'' = \bar{r}_i - \frac{1}{3}\sum_{k}^{1,3}\bar{r}_k$$

$$\bar{r}_j'' = \bar{r}_j - \frac{1}{2}\sum_{k}^{4,5}\bar{r}_k$$

$$\bar{R} = \frac{1}{3}\sum_{k}^{1,3}\bar{r}_k - \frac{1}{2}\sum_{k}^{4,5}\bar{r}_k$$

$$\bar{R}_{cm} = \frac{1}{5}\sum_{i}^{1,5}\bar{r}_i$$

This wavefunction is the product of a triton wavefunction, a deuteron wavefunction, the wavefunction which represents the relative motion between the deuteron and the triton, and the centre-of-mass motion wavefunction. In the notation used by several authors (1,6), this wavefunction would be designated by (123;45).

3.2 THE EXPANSION COEFFICIENTS

As in the case of the ground state calculation, the normalization constants for the cluster model and shell model wavefunction must first be calculated.

The complete normalized cluster model wavefunction before antisymmetrization may be represented by (1)

$$\Phi_{CM} = N_{CM}\,(123;45)\,\frac{1}{\sqrt{6}}\left[\{\alpha_1\beta_3 + \beta_1\alpha_3\}\alpha_2 - 2\alpha_1\beta_2\alpha_3\right]\alpha_4\alpha_5 \qquad ..(3\text{-}2)$$

which, when antisymmetrized, becomes

$$\begin{aligned} A\Phi_{CM} = \frac{N_{CM}}{4\sqrt{6}}\Big\{&[\beta_1\alpha_2 - \alpha_1\beta_2]\alpha_3\alpha_4\alpha_5\,[(123;45) - (124;35)] \\ &+ [\beta_2\alpha_5 - \alpha_2\beta_5]\alpha_1\alpha_3\alpha_4\,[(523;41) - (524;31)] \\ &+ [\beta_5\alpha_1 - \alpha_5\beta_1]\alpha_2\alpha_3\alpha_4\,[(153;42) - (154;32)]\Big\} \end{aligned} \qquad (3\text{-}3)$$

The complete shell model wavefunction has the same form as (3-2) and (3-3), before and after antisymmetrization, respectively (3). The details of the calculation of the normalization constants are given in Appendix A.

For the second excited state, Lee (3) has shown that the expansion coefficients may be expressed by

$$b_i = \frac{N_{SM_I}\ N_{CM}}{8}\ \langle (12345)_i | (123;45) - 2(124;35) + (524;31)\rangle \qquad \ldots(3\text{-}4)$$

3.3 THE OVERLAP INTEGRALS

i) The first configuration to be considered is $(1s)^3(1p)^2$. This is the lowest energy shell model configuration which is consistent with the spin and parity of the $3/2^+$ state. The spatial wavefunction for this configuration is

$$(12345) = \exp\left(-\frac{1}{2}\mu \sum_{i}^{1,5} r_i^{\,2}\right) \bar{r}_4.\bar{r}_5 \qquad (3\text{-}5)$$

The normalization constant appears in Appendix A.

In the single-particle representation, the direct integral in eq. (3-4) is

$$\langle (12345)_1 | (123;45)\rangle = \int \exp(-\varphi_1) r_4.r_5 [\tfrac{1}{9}(r_1^{\,2} + r_2^{\,2} + r_3^{\,2} + 2\bar{r}_1.\bar{r}_2 + 2\bar{r}_1.\bar{r}_3 + 2\bar{r}_2.\bar{r}_3) + \tfrac{1}{4}(r_4^{\,2} + r_5^{\,2} + 2\bar{r}_4.\bar{r}_5) \qquad \ldots(3\text{-}6)$$

(3-6) con't.

$$- \frac{1}{3} (\bar{r}_1 \cdot \bar{r}_4 + \bar{r}_1 \cdot \bar{r}_5 + \bar{r}_2 \cdot \bar{r}_4 + \bar{r}_2 \cdot \bar{r}_5 + \bar{r}_3 \cdot \bar{r}_4 + \bar{r}_3 \cdot \bar{r}_5) \; d\bar{r}_1 \, d\bar{r}_2 \, d\bar{r}_3 \, d\bar{r}_4 \, d\bar{r}_5$$

where $\varphi_1 = P(r_1^2 + r_2^2 + r_3^2) + Q(r_4^2 + r_5^2) + R(\bar{r}_1 \cdot \bar{r}_2 + \bar{r}_1 \cdot \bar{r}_3 + \bar{r}_2 \cdot \bar{r}_3) + S(\bar{r}_1 \cdot \bar{r}_4 + \bar{r}_1 \cdot \bar{r}_5 + \bar{r}_2 \cdot \bar{r}_4 + \bar{r}_2 \cdot \bar{r}_5 + \bar{r}_3 \cdot \bar{r}_4 + \bar{r}_3 \cdot \bar{r}_5) + T\bar{r}_4 \cdot \bar{r}_5$

$$P = \frac{3}{5} \mu + \frac{1}{3} \alpha + \frac{1}{15} \beta$$

$$Q = \frac{3}{5} \mu + \frac{1}{4} \bar{\alpha} + \frac{3}{20} \beta$$

$$R = - \frac{1}{3} \alpha + \frac{2}{15} \beta + \frac{1}{5} \beta$$

$$S = \frac{1}{5} (\mu - \beta)$$

$$T = - \frac{1}{2} \bar{\alpha} + \frac{3}{10} \beta + \frac{1}{5} \mu$$

The single-particle representation of the one-particle exchange integral is

$$\langle (12345) | (124;35) \rangle = \int \exp(-\varphi_2) \bar{r}_4 \cdot \bar{r}_5 \, [\frac{1}{9} (r_1^2 + r_2^2 + r_4^2 + 2\bar{r}_1 \cdot \bar{r}_2 + 2\bar{r}_1 \cdot \bar{r}_4 + 2\bar{r}_2 \cdot \bar{r}_4) + \frac{1}{4}(r_3^2 + r_5^2 + 2\bar{r}_3 \cdot \bar{r}_5) - \frac{1}{3}(\bar{r}_1 \cdot \bar{r}_3 + \bar{r}_1 \cdot \bar{r}_5 + \bar{r}_2 \cdot \bar{r}_3 + \bar{r}_2 \cdot \bar{r}_5 + \bar{r}_3 \cdot \bar{r}_4 + \bar{r}_4 \cdot \bar{r}_5) \; d\bar{r}_1 \, d\bar{r}_2 \, d\bar{r}_3 \, d\bar{r}_4 \, d\bar{r}_5 \qquad (3\text{-}7)$$

$$
\begin{aligned}
\text{where } \varphi_2 &= P(r_2{}^2 + r_4{}^2 + r_5{}^2) + Q(r_1{}^2 + r_3{}^2) \\
&+ R(\overline{r}_1\cdot\overline{r}_2 + \overline{r}_1\cdot\overline{r}_4 + \overline{r}_2\cdot\overline{r}_4) + S(\overline{r}_1\cdot\overline{r}_3 + \overline{r}_1\cdot\overline{r}_5 + \overline{r}_2\cdot\overline{r}_3 \\
&+ \overline{r}_2\cdot\overline{r}_5 + \overline{r}_3\cdot\overline{r}_4 + \overline{r}_4\cdot\overline{r}_5) + T\overline{r}_3\cdot\overline{r}_5
\end{aligned}
$$

The single-particle representation of the two-particle exchange integral is

$$
\begin{aligned}
\langle(12345)_1|(524;31)\rangle &= \int \exp(-\varphi_3)\overline{r}_4\cdot\overline{r}_5 \ \tfrac{1}{9}(r_2{}^2 + r_4{}^2 + r_5{}^2 \\
&+ 2\overline{r}_2\cdot\overline{r}_4 + 2\overline{r}_2\cdot\overline{r}_5 + 2\overline{r}_4\cdot\overline{r}_5) + \tfrac{1}{4}(r_1{}^2 + r_2{}^2 + 2\overline{r}_1\cdot\overline{r}_3) \\
&- \tfrac{1}{3}(\overline{r}_1\cdot\overline{r}_2 + \overline{r}_1\cdot\overline{r}_4 + \overline{r}_1\cdot\overline{r}_5 + \overline{r}_2\cdot\overline{r}_3 + \overline{r}_3\cdot\overline{r}_4 + \overline{r}_3\cdot\overline{r}_5) \\
&d\overline{r}_1\, d\overline{r}_2\, d\overline{r}_3\, d\overline{r}_4\, d\overline{r}_5 \qquad (3\text{-}8)
\end{aligned}
$$

$$
\begin{aligned}
\text{where } \varphi_3 &= P(r_2{}^2 + r_4{}^2 + r_5{}^2) + Q(r_1{}^2 + r_3{}^2) \\
&+ R(\overline{r}_2\cdot\overline{r}_4 + \overline{r}_2\cdot\overline{r}_5 + \overline{r}_4\cdot\overline{r}_5) + S(\overline{r}_1\cdot\overline{r}_2 + \overline{r}_1\cdot\overline{r}_4 + \overline{r}_1\cdot\overline{r}_5 \\
&+ \overline{r}_2\cdot\overline{r}_3 + \overline{r}_3\cdot\overline{r}_4 + \overline{r}_3,\overline{r}_5) + T\overline{r}_1\cdot\overline{r}_3
\end{aligned}
$$

The details of the method by which these integrals were evaluated appear in Appendix B. For all calculations involving the second excited state, there are thus three integrals. It is possible to cast these all into the same form, which for this particular configuration is

$$\frac{3\pi^{15/2}}{4E(1)\,[E(1)\;E(3)\;E(6)\;E(10)\;E(15)]^{3/2}}\left[5\,\frac{E(2)\;E(4)}{E(1)}+3\,\frac{E(5)}{E(3)}\right] \quad ..(3\text{-}9)$$

where the definition of the E's is given in Appendix C. The discussion of the numerical results appears in Chapter 5.

ii) The next configuration to be considered is $(1s)^2(1p)^2(2s)$. When describing the second excited state of ^{5}He by the cluster model, correlations between the nucleons are assumed. Whereas in the ground state there was only one multiparticle cluster, there are two in the present case, a deuteron and a triton cluster. With this particular configuration an attempt is made to study the correlations within the triton cluster. This is accomplished by assuming a configuration in which one of the three 1s nucleons is promoted to the 2s state, thus breaking the correlation between the three nucleons in the shell model. The smallness of the contribution of this configuration will indicate the strength of the correlation between the particles in the triton cluster. A single-particle representation of the spatial part of this wavefunction is

$$(12345)_2 = \exp\left(-\frac{1}{2}\sum_{i}^{1,5} r_i^2\right)\left(\frac{3}{2} - \mu r_1^2\right)\bar{r}_4 \cdot \bar{r}_5 \qquad (3\text{-}10)$$

The normalization constant appears in Table 5 of Appendix A. The details of the calculations for the other integrals appear in Appendix B. These integrals can be cast into

$$\frac{3\pi^{15/2}}{4E(1)\,[E(1)\;E(3)\;E(6)\;E(10)\;E(15)} \Bigg[\frac{3}{2}\Bigg\{\frac{5E(4)\;E(7)}{E(1)}$$

$$+\frac{3E(5)\;E(8)}{E(3)} + \frac{3E(9)}{E(6)}\Bigg\} - \mu\Bigg\{\frac{35}{2}\,\frac{(E(2))^2\;E(4)\;E(7)}{(E(1))^2}$$

$$+\frac{5}{2E(1)\;E(3)}\,[\;E(2)\;E(5)\;(3E(2)\;E(8) + 2E(7))$$

$$+\;E(4)\;(2E(2)\;E(8) + 3E(7))] + \frac{15}{2}\;\frac{E(5)\;E(8)}{(E(3))^2}$$

$$+\frac{15}{2}\;\frac{(E(2))^2\;E(9)}{E(1)\;E(6)} + \frac{4}{2}\;\frac{E(9)}{E(3)\;E(6)}\Bigg\}\Bigg] \qquad (3\text{-}11)$$

The numerical evaluation of this integral will be discussed in Chapter 5.

iii) Next consider the configuration $(1s)^3(1p)(2p)$. This is used to test the strength of the correlation between the two nucleons in the deuteron cluster of the cluster model wavefunction, as was done in the previous configuration with the triton cluster. The spatial part of this wavefunction is

$$(12345)_3 = \exp\left(-\frac{1}{2}\mu \sum_{i}^{1,5} r_i^2\right) \bar{r}_4 \cdot \bar{r}_5 \left(\frac{5}{2} - \mu r_5^2\right) \qquad (3\text{-}12)$$

The expression for the normalization constant for this state appears in Table 5 of Appendix A. Details of the evaluation of the other integrals are given in Appendix B. The integrals can be cast into the form

$$\frac{3\pi^{15/2}}{4E(1)\,[E(1)\,E(3)\,E(6)\,E(10)\,E(15)]^{3/2}} \left[\frac{5}{2} \left\{ \frac{5E(2)\,E(4)}{E(1)} + \frac{3E(5)}{E(3)} \right\} - \mu \left\{ \frac{3\ 5(E(2))^2\,E(4)}{(E(1))^2} + \frac{2\ 5E(2)}{2E(1)\,E(3)} \left[E(2)\,E(4) + E(5)\right] + \frac{15}{2}\,\frac{E(5)}{(E(3))^2} \right\} \right]$$

Numerical results are given in Chapter 5.

iv) The last configuration to be considered is $(1s)^3(2p)^2$. This represents the situation where the relative motion part of the cluster model wavefunction is in the next excited state. The single-particle representation of the spatial part of this wavefunction is

$$(12345)_4 = \exp\left(-\frac{1}{2}\mu \sum_{i}^{1,5} r_i^2\right)\bar{r}_4 \cdot \bar{r}_5 \left(\frac{5}{2} - \mu r_4^2\right) \left(\frac{5}{2} - \mu r_5^2\right) \qquad ..(3\text{-}14)$$

The expression for the normalization constant appears in Table 5 of Appendix A. The details of the evaluation of the other integrals are given in Appendix B. The integrals can be cast into the form

$$
\begin{aligned}
&\frac{3\pi^{15/2}}{4E(1)\,[E(1)\;E(3)\;E(6)\;E(10)\;E(15)]^{3/2}}\Biggl[\frac{25}{4}\Biggl\{\frac{5E(2)\;E(4)}{E(1)} \\
&+\frac{3E(5)}{E(3)}\Biggr\}-\frac{5}{2}\mu\Biggl\{\frac{35\;E(2)\;E(4)}{2(E(1))^2}\,[(E(2))^2+(E(4))^2] \\
&+\frac{25}{2E(1)\;E(3)}\,[(E(2)+E(4)\;E(5))\;(E(2)\;E(5)+E(4))] \\
&+\frac{15\;E(5)}{(E(3))^2}+\frac{25\;E(2)\;E(4)}{2\;E(1)\;E(6)}+\frac{6\;E(5)}{E(3)\;E(6)}\Biggr\} \\
&+\mu^2\Biggl\{\frac{315}{4}\left(\frac{E(2)\;E(4)}{E(1)}\right)^3+\frac{35\;E(2)\;E(4)}{4\;(E(1))^2\;E(3)}\,[5\;(E(2)\;E(5))^2 \\
&+11\;E(2)\;E(4)\;E(5)+5\;(E(4))^2]+\frac{25\;E(5)}{4\;E(1)\;(E(3))^2} \\
&[6\;(E(2)\;E(5))^2+11\;E(2)\;E(4)\;E(5)+6\;(E(4))^2] \\
&+\frac{105}{4}\left(\frac{E(5)}{E(3)}\right)^3+\frac{175}{4}\;\frac{(E(2))^3\;E(4)}{(E(1))^2\;E(6)}+\frac{5\;E(2)}{4\;E(1)\;E(3)\;E(6)} \\
&(E(2)\;E(5)+E(4))+\frac{75}{4}\;\frac{E(5)}{(E(3))^2\;E(6)}\Biggr\}\Biggr] \qquad (3\text{-}15)
\end{aligned}
$$

Again, numerical results appear in Chapter 5.

CHAPTER 4

NUMERICAL ANALYSIS AND DISCUSSION OF THE DECOMPOSITION PROBLEM

4.1 INTRODUCTION

This chapter will contain the numerical analysis and discussion of the decomposition of the ground state and second excited state cluster model wavefunctions into shell model wavefunctions.

The values of the cluster model width parameters for the ground state and second excited state cluster model wavefunctions as determined by Pearlstein et. al. in their variational calculations on the energies of these states appear in Table 1. The value of the width parameter for the shell model wavefunctions as determined by Feingold (8) is also shown in this table. These are the parameters used by Lee (3). When Pearlstein et. al. determined the parameters for the cluster model wavefunction, they found that two different spin-orbit forces gave equally good results in their variational calculation; this results in there

TABLE 1

CLUSTER MODEL AND SHELL MODEL PARAMETERS

PARAMETER	VALUE (fm^{-2})	DESCRIPTION
μ	0.365	SINGLE-PARTICLE
α'	0.433	INTERNAL ALPHA-PARTICLE
β'	0.225	GROUND STATE-RELATIVE
	0.325	
α	0.281	INTERNAL TRITON-PARTICLE
$\bar{\alpha}$	0.478	INTERNAL DEUTERON-PARTICLE
β	0.0422	SECOND EXCITED STATE RELATIVE

being two values for one of the parameters, β.

4.2 NUMERICAL ANALYSIS OF THE GROUND STATE CLUSTER MODEL WAVEFUNCTION

The closed form of the integrals given in Chapter 2 were coded and evaluated for several values of each parameter. The coefficients were evaluated first with each parameter equal to its value as given in Table 1; each parameter was then allowed to vary. Pearlstein et. al. (4) found that the energy was rather insensitive to small variations in the parameters. In this calculation, the parameters were allowed to vary to ascertain the sensitivity of the intensities to changes in the value of the parameters.

Table 2 gives the intensities of the different configurations contributing to the ground state cluster model wavefunction. These intensities were computed with the parameters equal to the value shown in Table 1. Coefficients for the configurations $(1s)^2(1p)^3$, $(1s)^2(1p)(2s)^2$ and $(1s)^3(1p)(3s)$ were calculated and each found to contribute less than 0.001%.

In Fig. 1, α' is held at its cluster model value of 0.433 fm^{-2} and the percentage contribution of

TABLE 2

SHELL MODEL CONTRIBUTIONS TO THE GROUND STATE

CONFIGURATION	INTENSITY (%)	
	$\beta' = 0.225$	$\beta' = 0.325$
$(1s)^4(1p)$	87.54	96.88
$(1s)^3(1p)(2s)$	0.22	0.46
$(1s)^4(2p)$	4.39	0.15
$(1s)^4(3p)$	0.33	0.02
TOTAL	92.49	97.49

the various configurations plotted as a function of β'. In Fig. 2, β' is held constant at 0.225 fm^{-2} and α' is varied. Fig. 3 is similar to Fig. 2 but with $\beta' = 0.325$ fm^{-2}. These figures will be discussed and evaluated in the next section.

4.3 DISCUSSION OF THE GROUND STATE DECOMPOSITION

As a check on the calculations, the parameters were all set equal to 0.365 fm^{-2}, the value of the shell model width parameter μ. In this case the contribution of the $(1s)^4(1p)$ configuration was found to equal 100%, and that for all other configurations to be zero. The significance of this is that when all the parameters in the cluster model wavefunction are set equal, this wavefunction is equivalent to the $(1s)^4(1p)$ shell model wavefunction (3). Since the shell model wavefunctions form an orthonormal set, then all the other configurations are orthogonal to this particular cluster model wavefunction.

The results and their implications will now be discussed. The first question to be answered is why the totals are less than 100%. Quite simply, an insufficient number of states was considered; the four states which on physical grounds should be most important

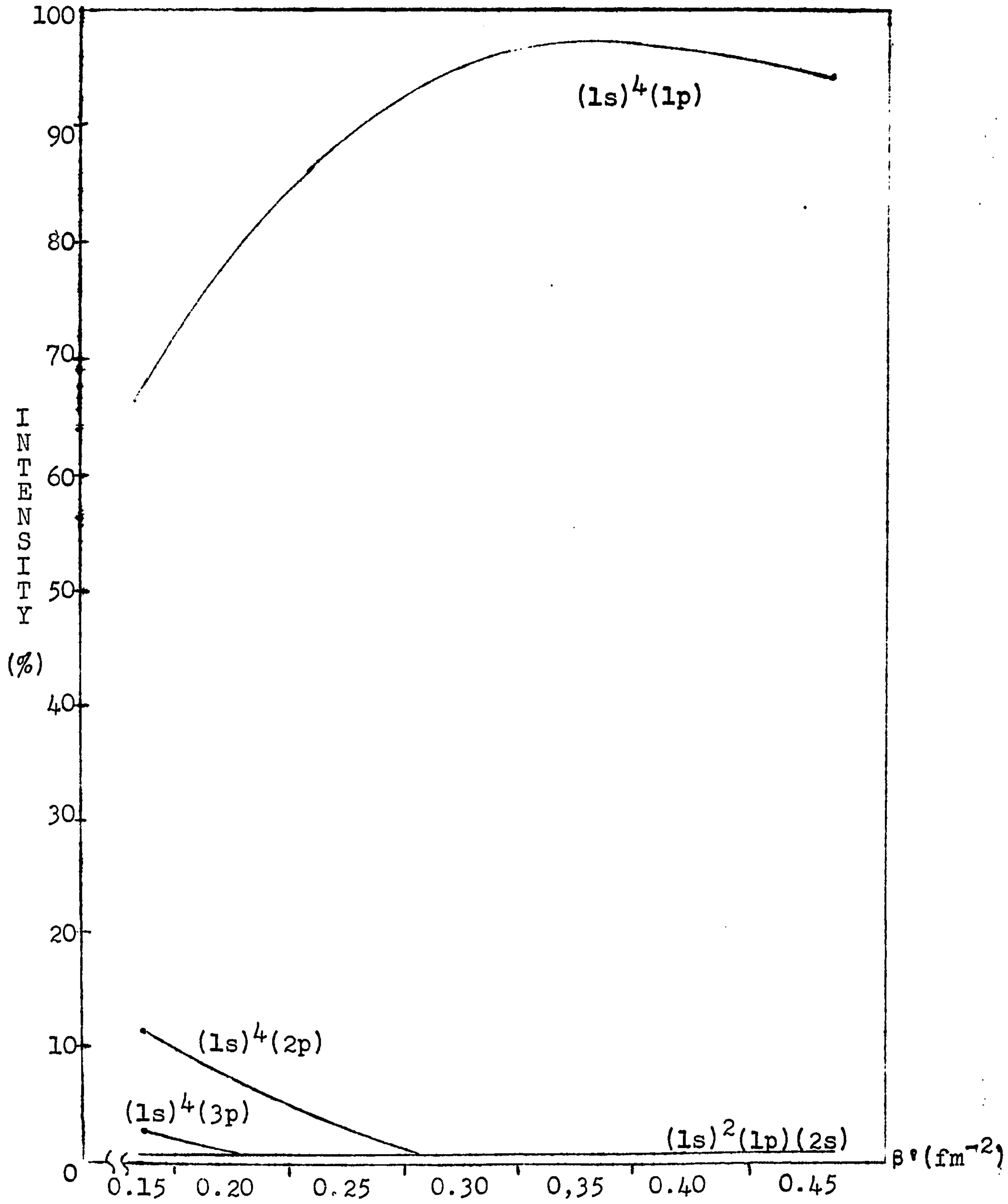


Fig. 1 Intensity versus β' with μ=0.365 fm^{-2} and α'=0.433 fm^{-2} for the Ground State.

have been taken into account, so that all the remaining states would probably individually contribute very little. Furthermore, it was not certain which other states should be considered to give the next largest contribution. Whether or not there remains a single configuration which makes a significant addition to the total is an open question. It must be remembered that in order to get the total greater than any predetermined number there is no a priori way of knowing which states are required.

Each shell model state will be considered individually. The first state to be considered is $(1s)^4(1p)$. This is the simple shell model representation of the $3/2^-$ state of ^{5}He. As seen in Figs. 1 and 2, it contributes to the cluster model wavefunction more than any of the other configurations. In Fig. 1, it is seen that the contribution is quite independent of the width parameter associated with the relative motion β', until it becomes smaller than 0.3 fm^{-2}, at which point this contribution drops rather drastically. As β' gets smaller, the separation between the neutron and the alpha-particle cluster increases, whereas in this shell model configuration the separation between nucleons is fixed by the parameter μ. Consequently, the contribution of this configuration decreases, and the contribution of a configuration in which the separation between

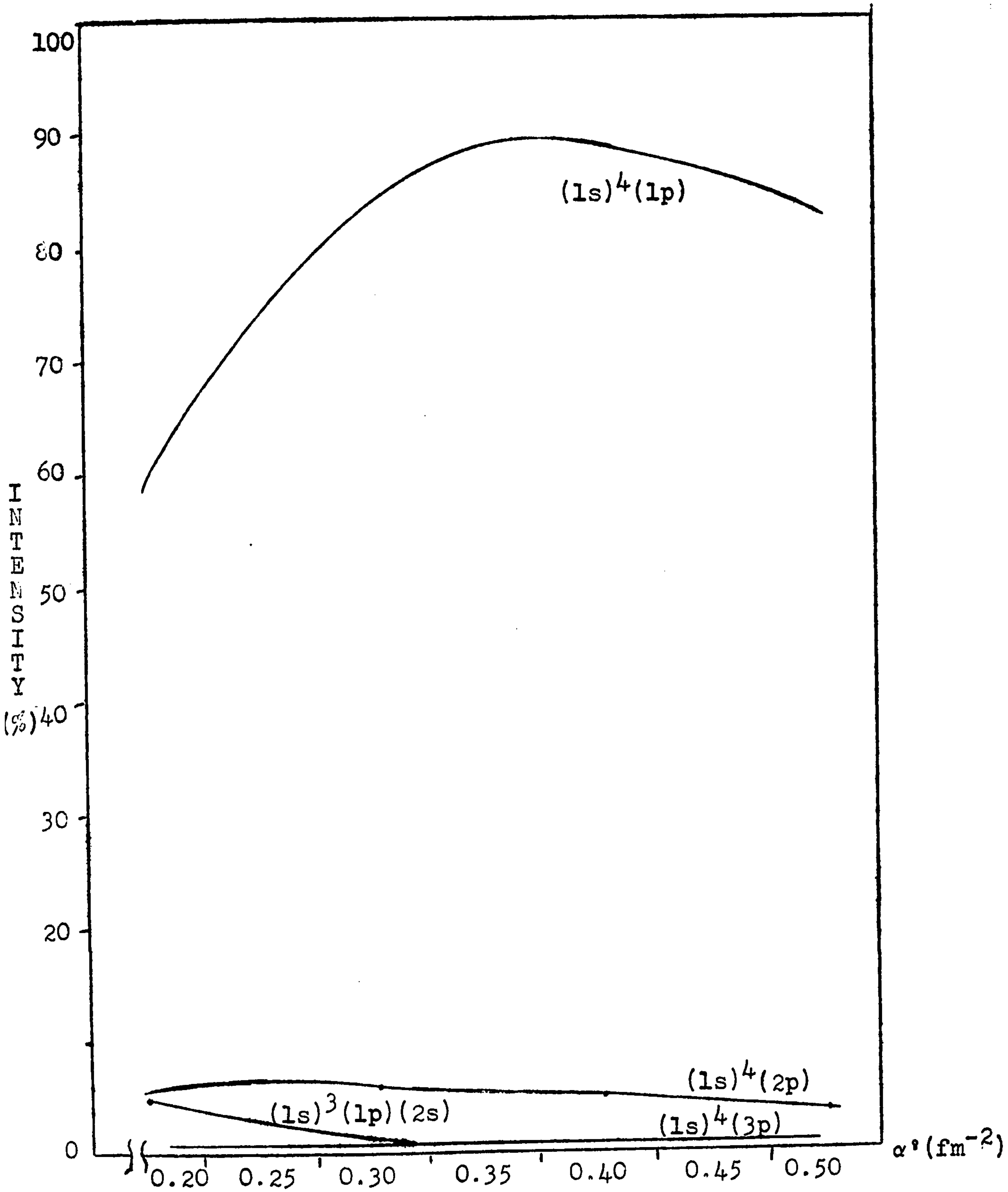


Fig. 2 Intensity versus α' with $\mu=0.365\ \mathrm{fm}^{-2}$ and $\beta'=0.225\ \mathrm{fm}^{-2}$ for the Ground State.

nucleons is greater (e.g. $(1s)^4(2p)$) increases. The $(1s)^3(1p)(2s)$ configuration, which represents the lowest energy excited state in which the alpha-particle cluster is broken up, is rather insensitive to the value of β'. It is always small. The $(1s)^4(2p)$ and $(1s)^4(3p)$ are most important when β' is small. This comes about because the separation between the neutron and the alpha-particle cluster is larger when β' is small, and in these configurations the neutron is far removed from the other nucleons. Thus three configurations have been considered in which one nucleon is removed from the other four to a varying degree. Also a configuration was considered which did not reflect in its shell structure the four-particle correlation intrinsic to the cluster model wavefunction.

In Fig. 2 it will be noticed that as α', the width parameter associated with the internal motion of the alpha-particle cluster, becomes smaller, the $(1s)^4(1p)$ and $(1s)^4(2p)$ contributions diminish, while the contribution of $(1s)^3(1p)(2s)$ increases. As α' decreases, the four-particle correlation decreases, so that contributions of configurations which describe this situation increase.

Fig. 3 is similar to Fig. 2 except that the value of β' is fixed at 0.325 fm^{-2}. This is closer to

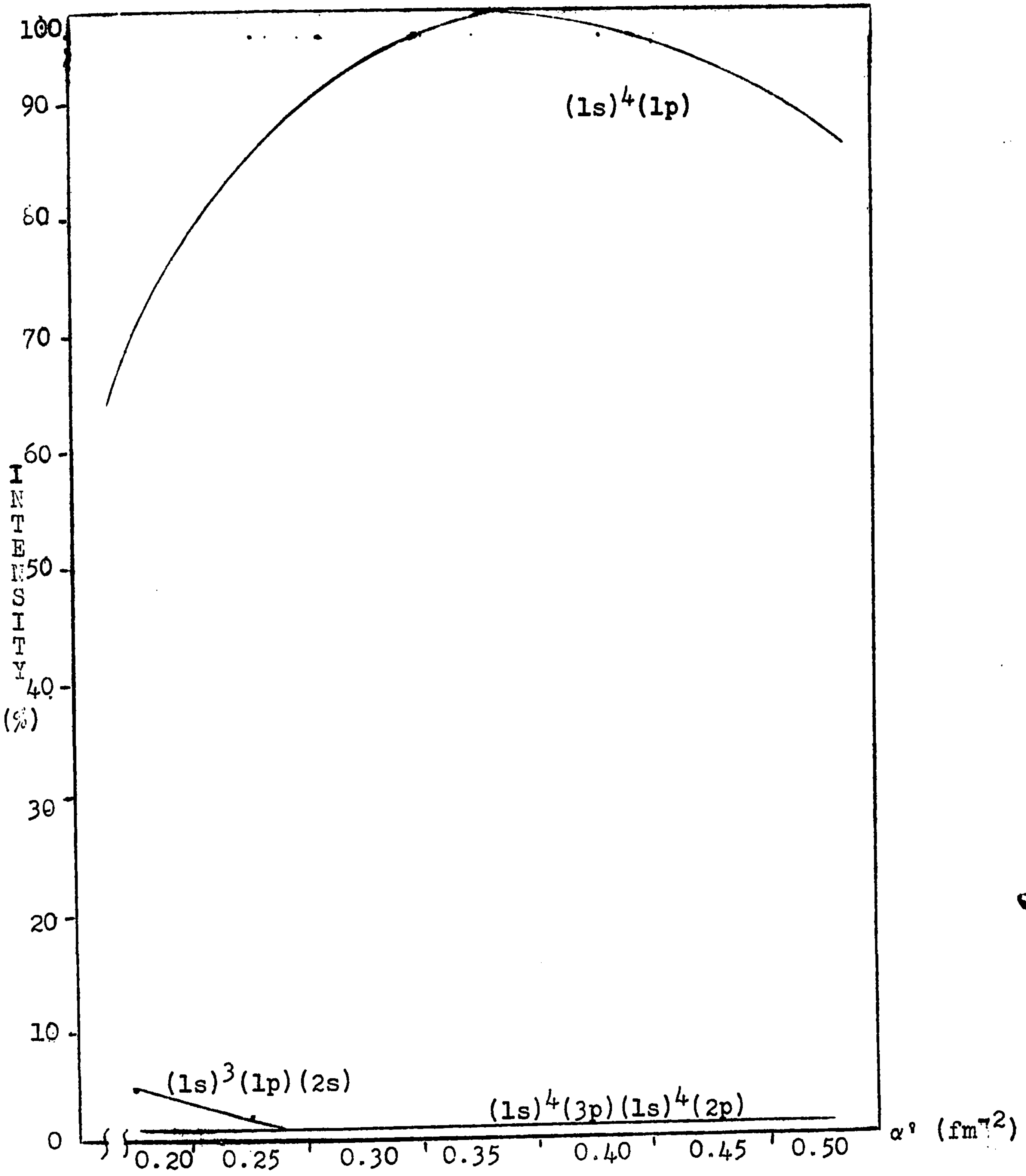


Fig. 3 Intensity versus α' with μ=0.365 fm^{-2} and β'=0.325 fm^{-2} for the Ground State.

the value of the shell model parameter, and hence the $(1s)^4(1p)$ configuration contributes much more; and all the other configurations contribute much less. Aside from this, the same general features of Fig. 2 are seen.

4.4 NUMERICAL ANALYSIS OF THE SECOND EXCITED STATE CLUSTER MODEL WAVEFUNCTION

As in the case of the ground state, the analytical expressions for the expansion coefficients were coded and evaluated for several values of each parameter. In Table 3 the intensities of the different configurations contributing to the cluster model wavefunction are presented, using the set of parameters found by Pearlstein et. al. (4) in their variational calculation of the energy of the second excited state.

The wavefunction of the second excited state involves three width parameters: β is related to the relative motion of the two clusters; α is the width parameter associated with the internal motion of the triton cluster; and $\bar{\alpha}$ is the width parameter associated with the internal motion of the deuteron cluster. In Figs. 4, 5 and 6 the intensities of all the configurations have been plotted as functions of one of these parameters.

TABLE 3

SHELL MODEL CONTRIBUTIONS TO THE SECOND EXCITED STATE

CONFIGURATION	INTENSITY (%)
$(1s)^3(1p)^2$	4.28
$(1s)^2(1p)^2(2s)$	0.94
$(1s)^3(1p)(2p)$	0.87
$(1s)^3(2p)^2$	0.48
TOTAL	6.57

4.5 DISCUSSION OF THE SECOND EXCITED STATE DECOMPOSITION

The first and most striking observation is that the four configurations considered add up only to 6.57%. Yet from shell model considerations, it would be concluded that these configurations should play a more important part in describing the cluster model wave-function than they appear to do. The main reason for the failure of the simple shell model argument to predict the most important configuration is the relative size of the cluster model parameter, ρ, as determined by Pearlstein et. al. (4).

In the ground state calculation, the value of the largest parameter is less than twice the size of the smallest parameter. Consequently, the reasoning behind the selection of the important shell model configurations is relatively straightforward. In the present case, the value of the largest parameter is greater than that of the smallest by an order of magnitude. Thus, the reasoning for the shell model configuration selection is not as simple. Obviously, higher energy states must be taken into account, although it is not clear which will be the most important.

In Fig. 4 the intensities are plotted as functions of the width parameter of the relative motion wavefunction. The $(1s)^3(1p)^2$ contribution increases monotonically quite rapidly with increasing β. This is to be expected since as β comes closer to the value of the shell model parameter, the shell model prediction of the most important configuration should become more applicable.

The behaviour of the remaining three configurations have features similar to one another. They all contribute very little when β has the value shown in Table 1. As β increases, their contribution first increases, then decreases, until β is equal to the shell model value, when the contribution is again small.

As β is varied, the separation between clusters and hence between some nucleons change. When these distances correspond to the inter-nucleon distances of any shell model configuration, the intensity of that particular configuration increases. As higher energy configurations are considered the position of this increase moves to lower values of β. It might be concluded that for some configuration its maximum would occur when β has the value in Table 1. As higher energy

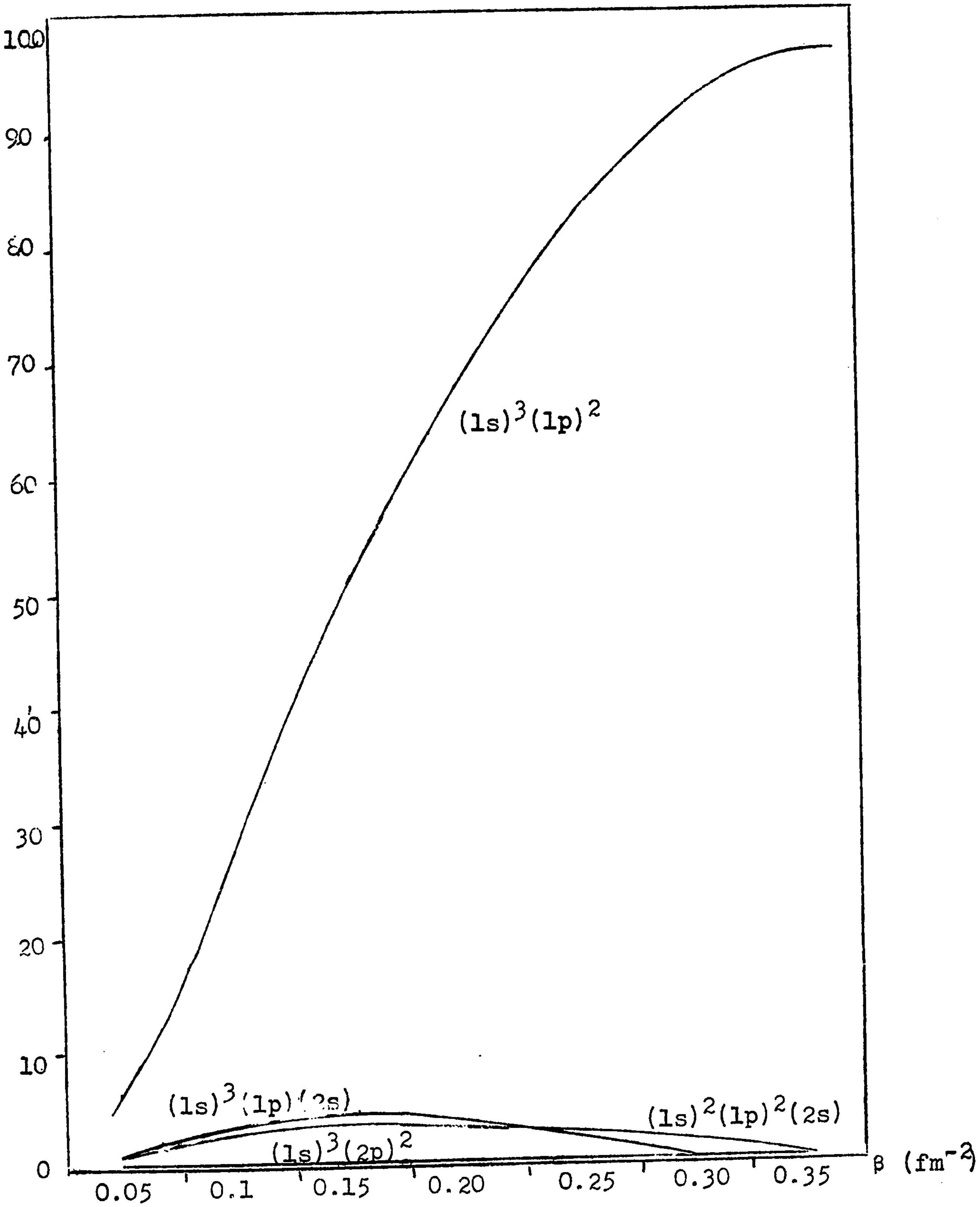
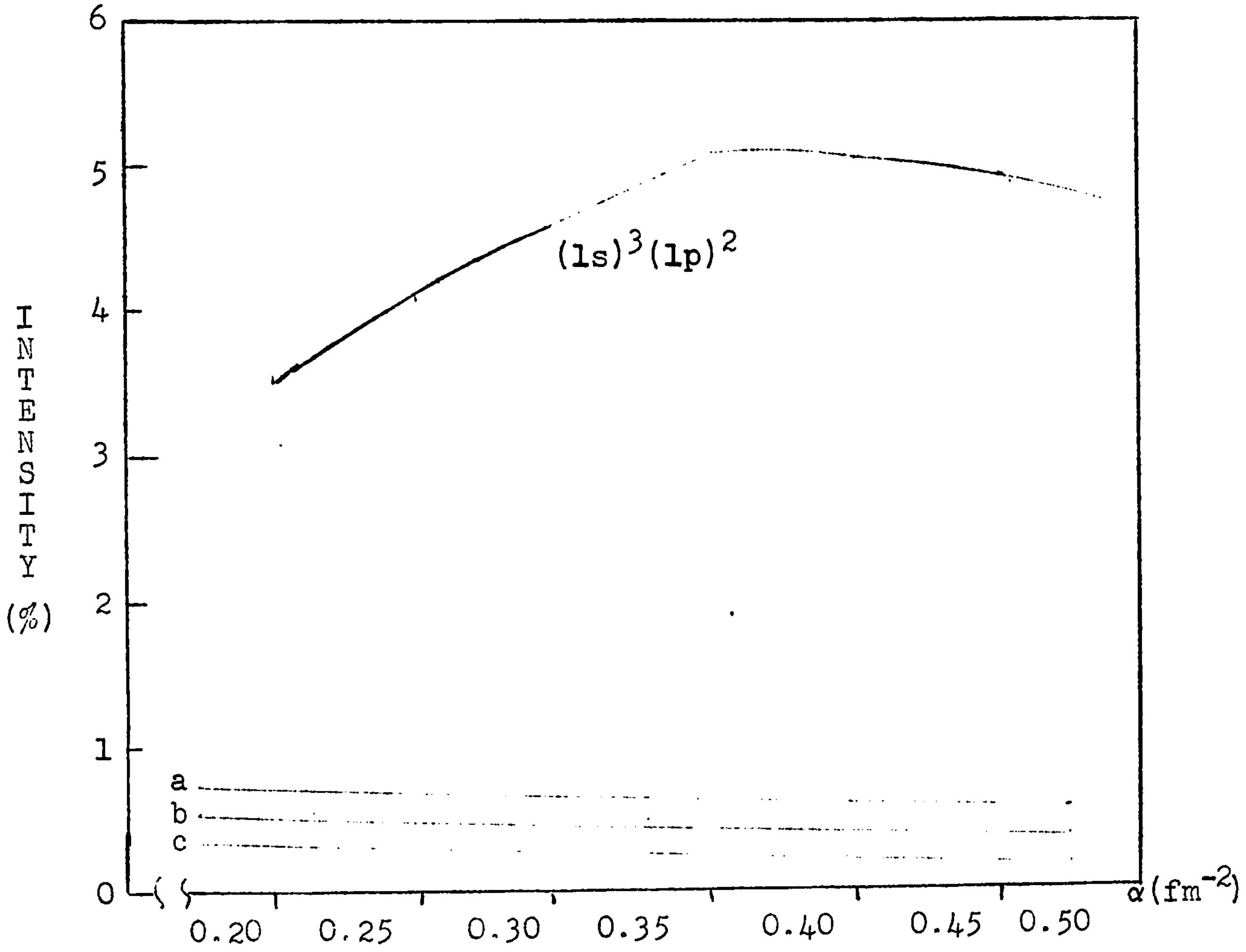


Fig. 4 Intensity versus β with $\mu=0.365\ fm^{-2}$, $\alpha=0.281\ fm^{-2}$ and $\bar{\alpha}=0.478\ fm^{-2}$ for the Second Excited State.

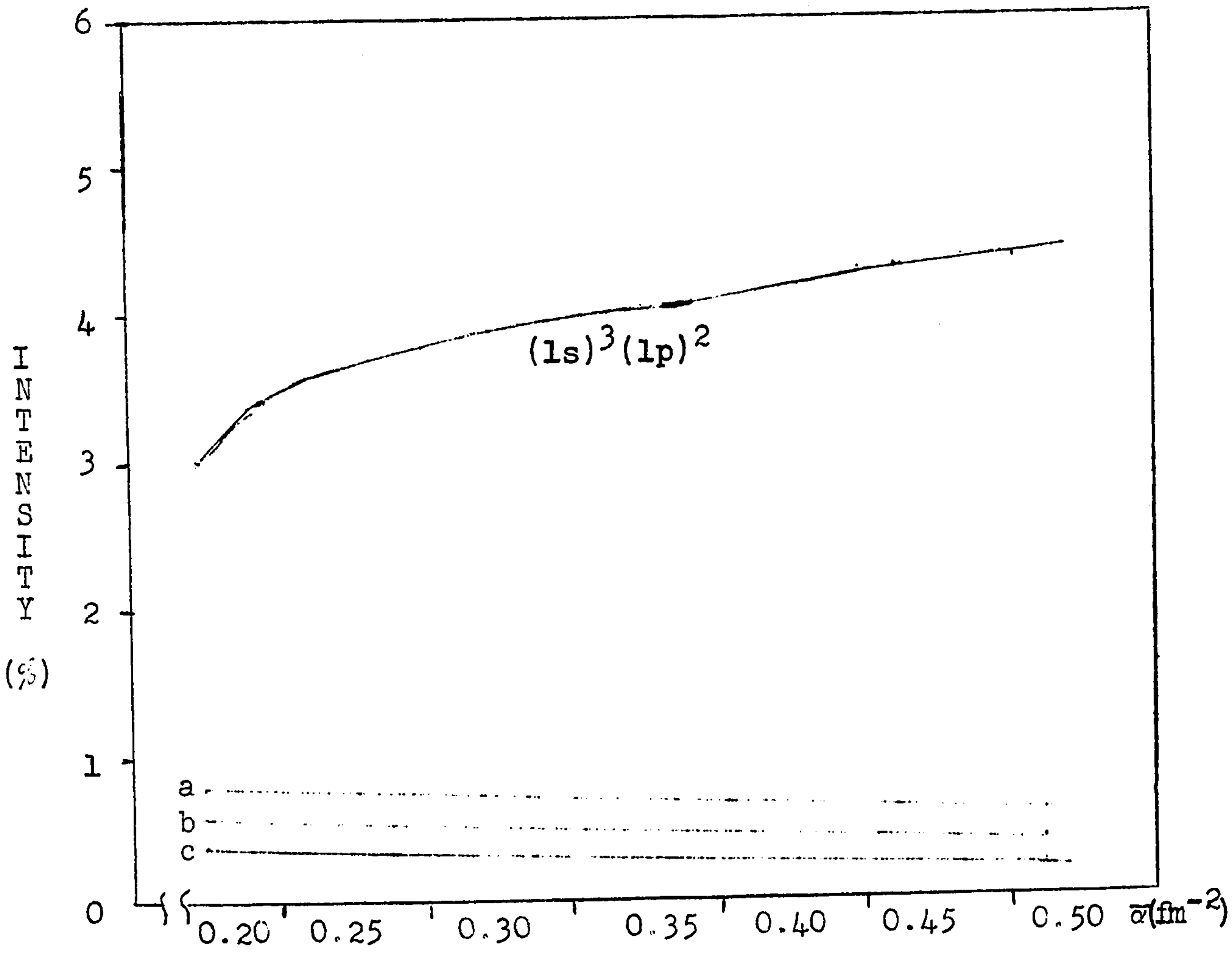
configurations are considered, however, their contributions appear to bcome smaller than those of lower energy configurations. There appears no simple way to find any configurations to solve this difficulty.

In the two figures in which β is held constant, Figs. 5 and 6, the intensities remain almost constant as α and $\bar{\alpha}$ are varied. There are two possible explanations for this: either the intensities are not very sensitive to the size of the clusters, or the small value of β dominates every other possible effect. The implication of the latter explanation is that since the intensities are themselves intrinsically small, any variation in them must also be small in absolute value.



a = $(1s)^2(1p)^2(2s)$
b = $(1s)^3(1p)(2p)$
c = $(1s)^3(2p)^2$

Fig. 5 Intensity versus α with $\mu = 0.365\ \mathrm{fm}^{-2}$, $\beta=0.0422$, $\bar{\alpha}=0.478$ for Second Excited State.



a = $(1s)^2(1p)^2(2s)$
b = $(1s)^3(1p)(2p)$
c = $(1s)^3(2p)^2$

Fig. 6 Intensity versus $\bar{\alpha}$ with $\mu=0.365$ fm^{-2}, $\beta=0.0422$, $\alpha=0.281$ for the Second Excited State.

CHAPTER 5

ADDITIONAL CALCULATIONS ON THE FIRST EXCITED STATE OF ^{5}He

5.1 INTRODUCTION

This chapter will be concerned with the derivation of the formalism used in an attempt to find a suitable set of width parameters for the cluster model wavefunction representing the first excited $(\frac{1}{2}^-)$ state of ^{5}He. This state is assumed to have the same cluster configuration as the ground state, i.e. alpha-particle and a neutron.

The radiative transition probability from the second excited state to the first excited state is computed for several values of each parameter; the same is done for the energy matrix element of the $\frac{1}{2}^-$ state. The calculated values are then compared with the experimental results to determine if a set of parameters consistent with both energy and radiative width can be found to describe this particular state.

5.2 THE CLUSTER MODEL WAVEFUNCTION

The cluster configuration used to describe this state is the same as that used to describe the ground state. The spatial part of the wavefunction is given by eq. (2-1); the spin wavefunction is constructed in the following.

The total spin and parity of the nucleus in this state is $\frac{1}{2}^-$. The first excited state of ^{5}He has an orbital angular momentum L = 1 for the relative motion of the two clusters. Hence coupling a spin of $\frac{1}{2}$ to the angular momentum 1 gives a total angular momentum of $J = \frac{1}{2}$.

$$|JM\rangle = \sum_{m_S + m_L = M} |SM_s\rangle |LM_L\rangle \langle SLM_sM_L|JM\rangle \qquad (5\text{-}1)$$

$$|\tfrac{1}{2}\,\tfrac{1}{2}\rangle = \sqrt{\tfrac{2}{3}}\,|11\rangle|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle_s - \sqrt{\tfrac{1}{3}}\,|10\rangle|\tfrac{1}{2}\,\tfrac{1}{2}\rangle_s$$

$$|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle = \sqrt{\tfrac{1}{3}}\,|10\rangle\tfrac{1}{2}\,-\tfrac{1}{2}\rangle_s - \sqrt{\tfrac{2}{3}}\,|1\,-1\rangle|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle_s \qquad (5\text{-}2)$$

where $|\tfrac{1}{2}\,\tfrac{1}{2}\rangle_s = \alpha_1\beta_2\alpha_3\beta_4\alpha_5$

$|\tfrac{1}{2}\,-\tfrac{1}{2}\rangle_s = \alpha_1\beta_2\alpha_3\beta_4\alpha_5$

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

To obtain the complete wavefunction, all functions in eq. (5-2) must be multiplied by the internal cluster model wavefunction and the radial part of the wavefunction associated with the relative motion. The complete wavefunctions are

$$\Phi(+\tfrac{1}{2}) = \sqrt{\tfrac{2}{3}}\,(1234;5)_{M_L = 1}\ \alpha_1\beta_2\alpha_3\beta_4\beta_5 - \sqrt{\tfrac{1}{3}}\,(1234;5)_{M_L = 1}\ \alpha_1\beta_2\alpha_3\beta_4\alpha_5 \tag{5-3}$$

$$\Phi(-\tfrac{1}{2}) = \sqrt{\tfrac{1}{3}}\,(1234;5)_{M_L = 0}\ \alpha_1\beta_2\alpha_3\beta_4\beta_5 - \sqrt{\tfrac{2}{3}}\,(1234;5)_{M_L = 1}\ \alpha_1\beta_2\alpha_3\beta_4\alpha_5 \tag{5-4}$$

It should be noted that these wavefunctions are orthogonal to the ground state wavefunction, due to the fact that they are states of opposite parity.

5.3 TRANSITION PROBABILITY

The normalization constant for the second excited state has been calculated in Appendix A. It is easily shown that the same definition of the normalization constant holds for the first excited state, although the spin wavefunction is different.

Next the calculation of the transition matrix element itself will be considered. The transition probability for the emission of a photon with energy, $\hbar\omega$, angular momentum λ, μ, and of electric or magnetic multipolarity, in which the nucleus goes from a state i to a state f, is (9)

$$T_{if}\ (\sigma\lambda) = \frac{8\Pi\ (\lambda + 1)}{\lambda[\,(2\lambda + 1)!!]^2}\ \frac{\kappa^{2\lambda + 1}}{\hbar}\ B(\sigma\lambda) \qquad (5\text{-}5)$$

where $B(\sigma\lambda,\ J_i - J_f)$ is the reduced matrix element

$$B(\sigma\lambda,\ J_i \rightarrow J_f) = \frac{1}{2J_i + 1} \sum_{M_i M_f} |\langle f|Q_{\lambda\mu}|i\rangle|^2 \qquad (5\text{-}6)$$

$Q_{\lambda\mu}$ is the electric multipole operator, where

$$Q_{\lambda\mu} = \sum_i e_i r_i^{\lambda}\ Y_{\lambda}^{\mu *}\ (\Omega_i) - i\ \mu_o \kappa(\lambda + 1)^{-1} \sum_i g_{si} \vec{\sigma}_i \times \vec{r}_i \cdot \nabla\ (r^{\lambda}\ Y_{\lambda}^{\mu *})_i \qquad (5\text{-}7)$$

Since here $\Pi_i = \Pi_f = -1$, $J_i = 3/2$, $J_f = 1/2$, the radiation must be of odd parity and

$$\lambda = |J_i - J_f| = 2 \text{ or } 1$$

Since the lowest order non-zero term is in general much larger than any higher order term, $\lambda = 2$ can be neglected, so that this is an E1 transition. Eq. (5-5) and (5-6) reduce in this case to

$$T_{if}\ (E1) = \frac{16\Pi}{9}\ \frac{\kappa^3}{\hbar}\ B(E1)$$

$$B(E1,\ \tfrac{3}{2} \rightarrow \tfrac{3}{2}) = \frac{1}{4} \sum_{M_i M_f} |\langle f|Q_{1\mu}|i\rangle|^2 \qquad (5\text{-}8)$$

respectively.

The **selection rule for radiative transitions** requires that only one value of μ contribute to each term of the sum in eq. (5-8)

$$\mu = M_i - M_f \quad (\mu = 0, 1, -1) \tag{5-9}$$

As the matrix element of the second term of the electric dipole operator is much smaller than that of the first term, it is neglected in the calculation of T(E1). The dipole operator reduces to

$$Q_{1\mu} \simeq e R_{1\mu}$$

where

$$R_{1\mu} = \sum_{i}^{3,4} r_i Y_i^{\mu *} (\Omega_i) \tag{5-10}$$

The terms in eq. (5-8) which contribute to B(E1) must be ascertained, subject to two conditions:

i) the selection rule (5-9)

ii) the spin configuration of the initial and final states must be identical.

Table 4 gives those terms which yield a non-zero contribution. Thus performing the sum in eq. (5-8) explicitly,

TABLE 4

NON-ZERO ELEMENTS CONTRIBUTING TO THE DIPOLE EXPECTATION VALUE

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

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

$$+ |\langle \Phi_f(-\tfrac{1}{2}) | R_{11} | \varphi_i(\tfrac{1}{2}) \rangle|^2 + |\langle \Phi_f(-\tfrac{1}{2}) | R_{10} | \varphi_i(-\tfrac{1}{2}) \rangle|^2 \} \tag{5-11}$$

After summing over the spins, the remaining spatial part of each term in eq. (5-11) reduces to

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

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

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

$$\langle \Phi_f(-\tfrac{1}{2}) | R_{10} | \varphi_i(-\tfrac{1}{2}) \rangle = \frac{N_i N_f}{6\sqrt{6}} \langle (5234;1)_0 - (1234;5)_0 | R_{10} | (123;45) \rangle . \tag{5-12}$$

Define I_k by (1)

$$I_k = (-)^k \langle (1234;5)_k - (5234;1)_k | R_{1-k} | (123;45); \tag{5-13}$$

then eq. (5-7) becomes

$$T(E1) = \frac{\Pi}{243} \frac{\kappa^3}{h} e^2 N_i^2 N_f^2 \{ |I_0|^2 + |I_1|^2 + |I_{-1}|^2 \} . \tag{5-14}$$

The numerical evaluation of this expression will be discussed in the next chapter.

5.4 ENERGY OF THE STATE

In this section the expectation value for the Hamiltonian will be evaluated. The state used will be the normalized cluster model wavefunction describing the first excited state of ^{5}He. The Hamiltonian used is that of Pearlstein et. al. (4) The potential operator

$$V_{ij} = - V_0 \exp(-\kappa r_{ij}^2) \{w(1 + P_{ij}^s) + b(P_{ij}^\sigma - P_{ij}^\tau)\}$$

$$- V_{LS} \exp(-\lambda r_{ij}^2) (r_i - r_j) \times (P_i - P_j) . (\sigma_i + \sigma_j)/2\hbar \tag{5-15}$$

where $V_0 = 68.6$ MeV, $\kappa = 0.416$ fm^{-2}, $w = 0.41$, $b = 0.09$,

$V_{LS} = 4.5$ MeV when $\lambda = 0.265$ fm^{-2}

$V_{LS} = 13.8$ MeV when $\lambda = 0.416$ fm^{-2}

and P_{ij}^s, P_{ij}^σ, P_{ij}^τ represent the space, spin and isobaric spin exchange operators, respectively. The two values of V_{LS} corresponds to the two different spin-orbit forces used by Pearlstein.

Pearlstein (4) has shown that the expectation value of the kinetic energy operator is

$$\langle T \rangle = \left(\frac{\hbar^2}{2M}\right) (5\beta' + 9\alpha') - \frac{\hbar N^2}{2M} \int (\Psi_0 - \Psi_1)^* \left(- 2\alpha'^2 \frac{\partial}{\partial \alpha'} - 2\beta' \frac{\partial}{\partial \beta'}\right) \Psi_0 \, d\tau . \tag{5-16}$$

where $\Psi_0 = (1234;5)$

$\Psi_1 = (5234;1)$

For potential operator, he gives

$$\langle V\rangle = \langle V_c\rangle + \langle V_{s0}\rangle$$

$$= N^2\{\int\Psi_0{}^*[w(12F_{12} + 3F_{15})]\Psi_0\, d\tau - \int\Psi_1{}^*[w\,(12F_{12}$$

$$+ 6F_{23} - 3F_{15})]\Psi_0\, d\tau\} + 2N^2\{\Psi_0{}^*(2G_{15}\Psi_0\, d\tau$$

$$- \int\Psi_1{}^*\,(G_{15} + G_{25})\Psi_0\, d\tau\}$$

$$F_{ij} = V_0 \exp(-\kappa\, r_{ij}{}^2)$$

$$G_{ij} = [V_{LS} \exp(-\lambda r_{ij}{}^2)\,(r_i - r_j)\,(P_i - P_j)]_z\, \hbar^{-1}$$

(5-17)

The numerical evaluation of these expectation values will be discussed in the next chapter.

CHAPTER 6

RESULTS AND DISCUSSION OF THE CALCULATION ON THE FIRST EXCITED STATE

6.1 NUMERICAL ANALYSIS OF THE TRANSITION PROBABILITY

It was shown in Chapter 5 that the calculation of the transition probability for the radiative decay of the second excited state to the first excited state could be cast into the same form as that from the second excited state to the ground state, previously performed by Tran Duc (1). His analysis was coded, and the transition probability was computed for various values of the cluster model width parameters used to describe the first excited state. In Fig. 7 the transition probability is plotted as a function of the parameters. In Figs. 8 and 9 the ratio of the transition probability from the ($3/2^+$) state to the ($3/2^-$) state, (1) to the transition probability from the ($3/2^+$) state to the ($1/2^-$) state is plotted as a function of the parameters.

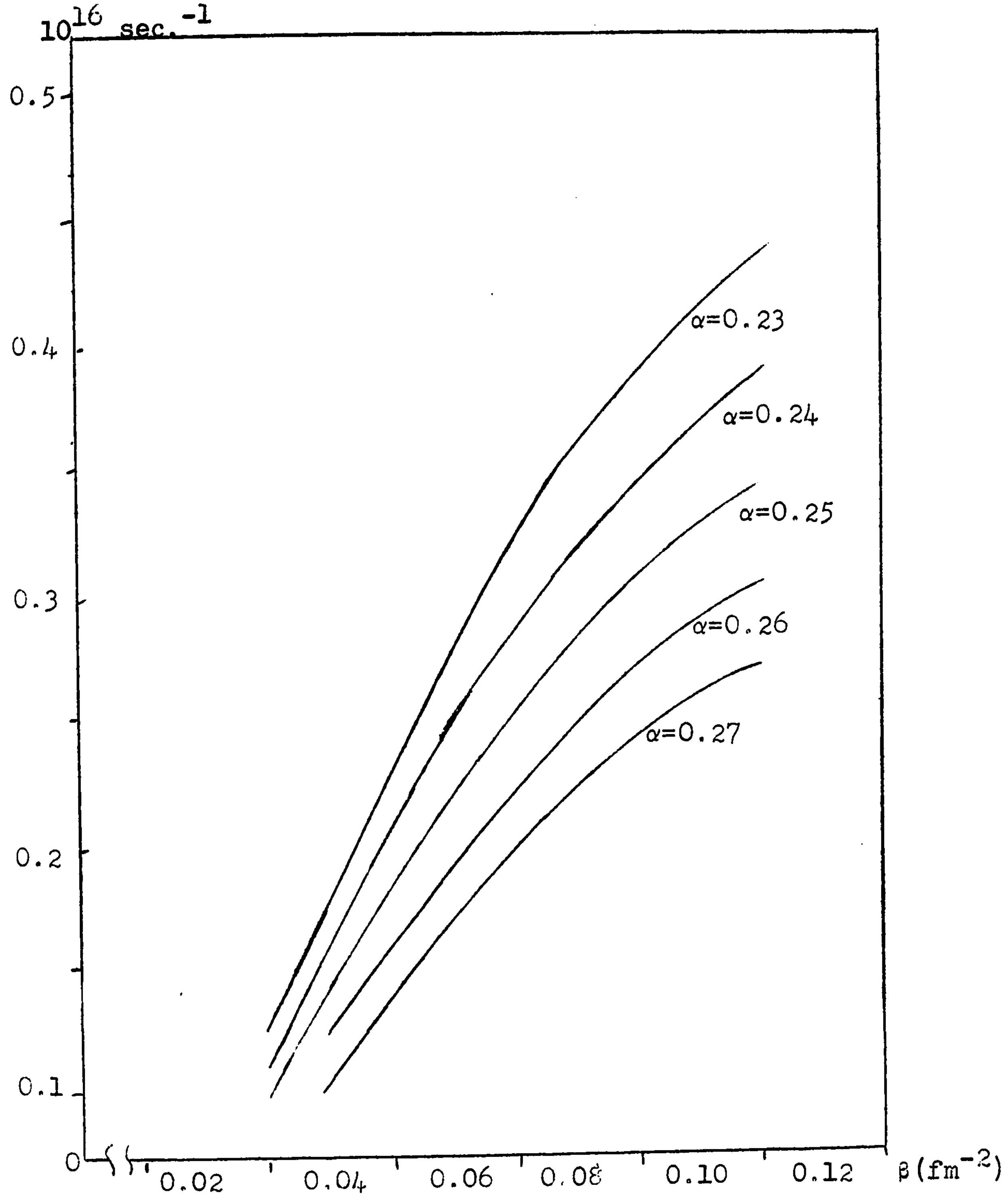


Fig. 7 Transition Probability versus The Relative Parameter for Several values of the Internal Parameter α. Note that both α and β are Expressed in units of fm^{-2}.

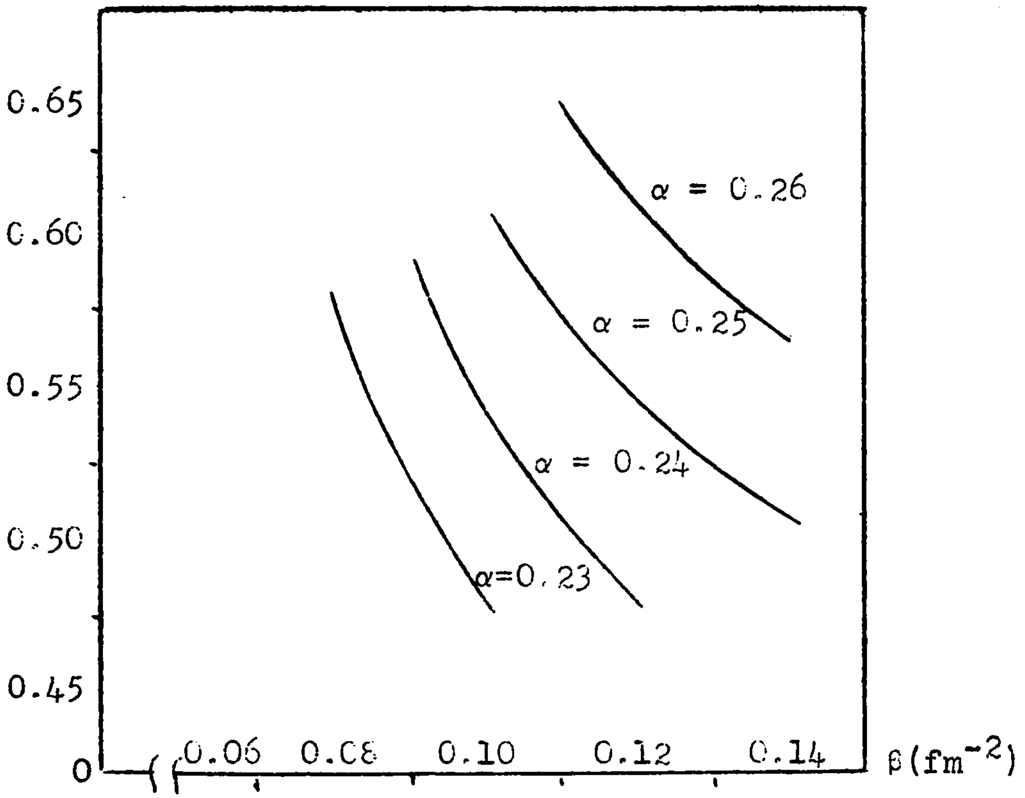


Fig. 8 Ratio of Transition Probability versus relative motion parameter using the value of 0.185 x 10^{16}sec^{-1} for the Probability to the Ground State.

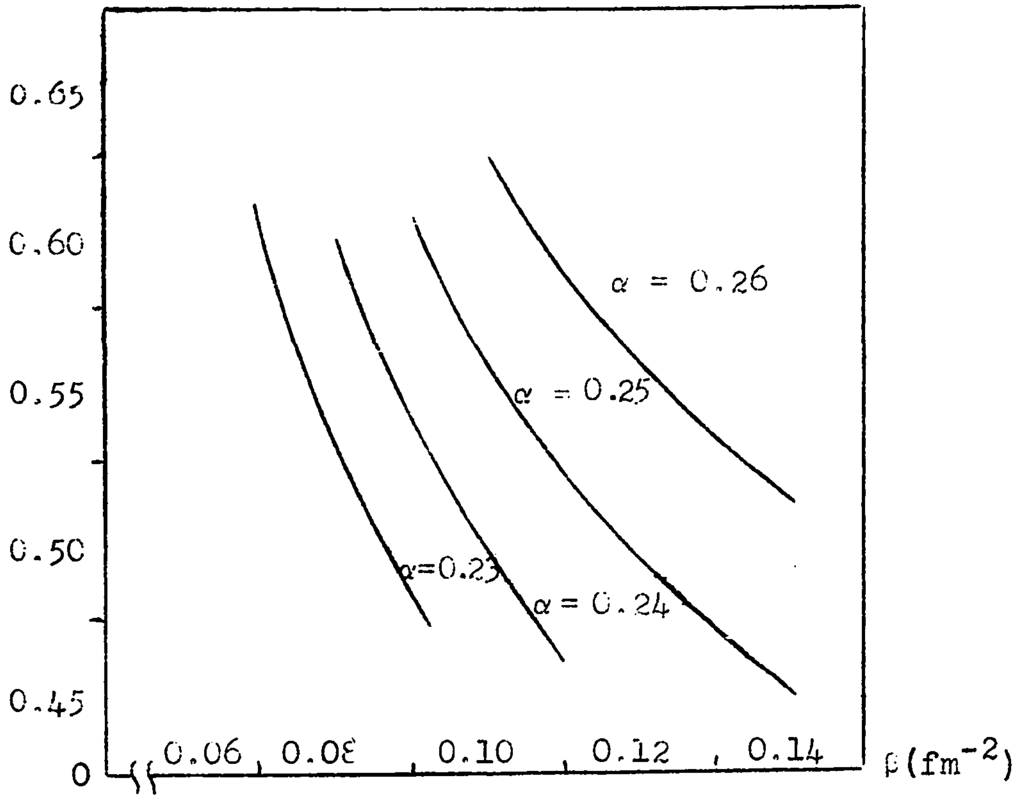


Fig. 9 Similar to Fig. 8, except the value of 0 172 x 10^{16}sec^{-1} is used for the Transition Probability to the Ground State.

6.2 NUMERICAL ANALYSIS OF THE ENERGY MATRIX ELEMENT

The analysis for the expectation value of the Hamiltonian appears in reference (4). This analysis was coded and evaluated for several sets of width parameters.

The process used to calculate the excitation of this state involves several steps. First, values of α and β in the wavefunction of the first excited state are selected. Second, using these parameters, the expectation value is computed; the result will be called the interaction energy. Third, β is set equal to zero, the expectation value is recalculated and subtracted from the interaction energy. The result is the interaction energy less the internal energy of the alpha-cluster using the potential given by eq. (5-15). Mang and Wild (10), using a more realistic force, have calculated the internal energy of an alpha-particle as a function of the width parameter appearing in its wavefunction. Their result is

$$E_{\alpha} = - 28.3 + 33.4(1 - 0.96/y)^2 \text{ MeV} \qquad (6\text{-}1)$$

where

$x = \beta/\alpha$
$y = \kappa/\alpha$
$\kappa = 0.416 \text{ fm}^{-2}$

The final step in the calculation of the excitation of this state is to add the internal energy of the alpha-cluster, as calculated from the expression given by Mang and Wild, to the interaction energy of the neutron with the alpha-cluster.

Figs. 10 and 11 show the plots of the excitation energy of the state as a function of the cluster model parameters for the two different spin-orbit forces used in Pearlstein's original calculation.

6.3 DISCUSSION

Buss et. al.(5) have measured the ratio of the transition probability from the second excited state to the ground state, to the transition probability from the second excited state to the first excited state and quote a value of 0.55. Tran Duc (1) using the results of Coon and Davis (11), estimated the radiative width of the transition to the ground state to be 1.3 eV. The calculation of Tran Duc (1) yields values of 1.23 eV and 1.12 eV for this width, corresponding to the two values of β' quoted by Pearlstein et. al. (4).

The excitation energy of the first excited state was measured by Fessenden and Maxson (12) to be

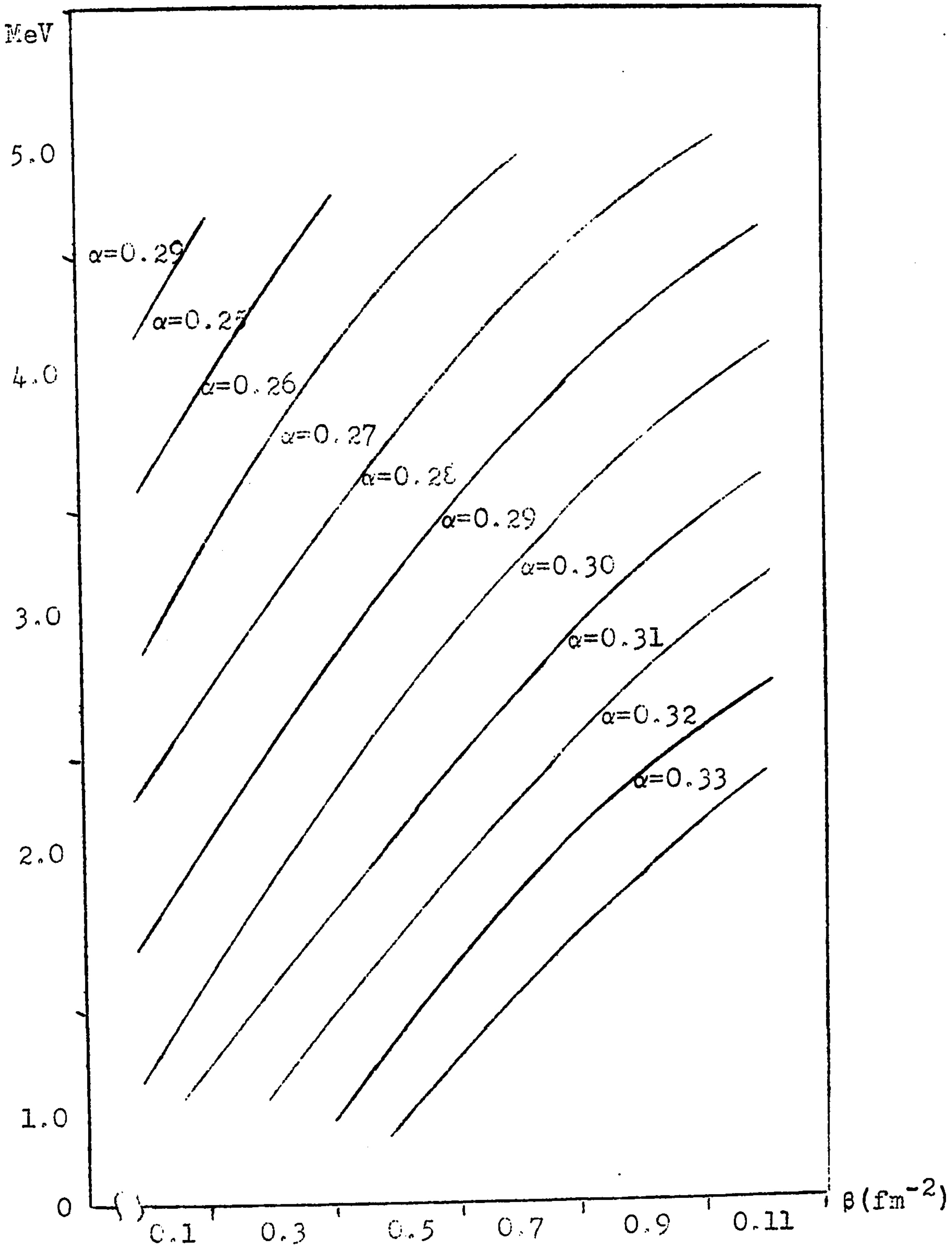


Fig. 10 Excitation Energy of the $1/2^-$ State as a Function of the Relative Parameter, calculated using spin orbit force with V_{LS}=4.5 MeV and λ=0.2657 fm^{-2}.

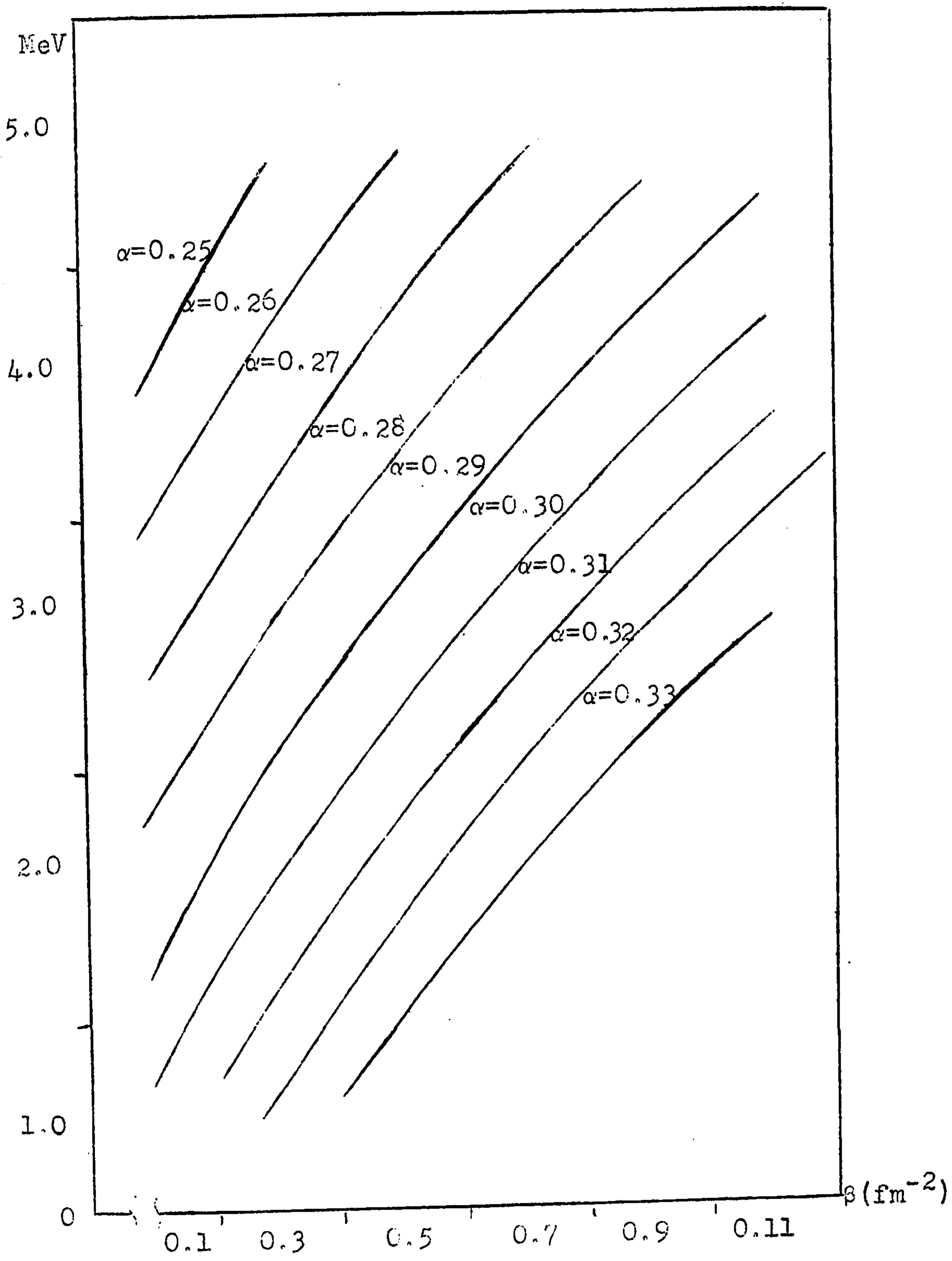


Fig. 11 Excitation Energy of the $1/2^-$ State as a Function of the Relative Parameter, calculated using spin orbit force with V_{LS}=13.8 MeV and λ= 0.416 fm^{-2}.

2.6 MeV. The choice of the cluster model parameters was restricted so as to yield the experimentally measured transition probability and the excitation energy for this state.

It was impossible to find such a set of parameters. Fig. 12 shows part of the α - β plane on which are indicated those values of the parameters which yield values of the energy and transition probability **within** 10% of measured values. No set of the parameters satisfies both criteria.

Some of the reasons for this lack of success are as follows. First consider the energy calculation. The kinetic energy part of the Hamiltonian is a gradient operator. The largest contribution to its expectation value comes from the region of configuration space where the single-particle coordinates assume small values. Similarly, since the potential operator contains an exponential function, the greater part of its contribution arises from small r. Since the most important contribution to the expectation value of the Hamiltonian thus arises from small values of r, the behaviour of the wavefunction in this region is most important to the Hamiltonian. The wavefunction gives the correct value for the energy when β is small, and α large.

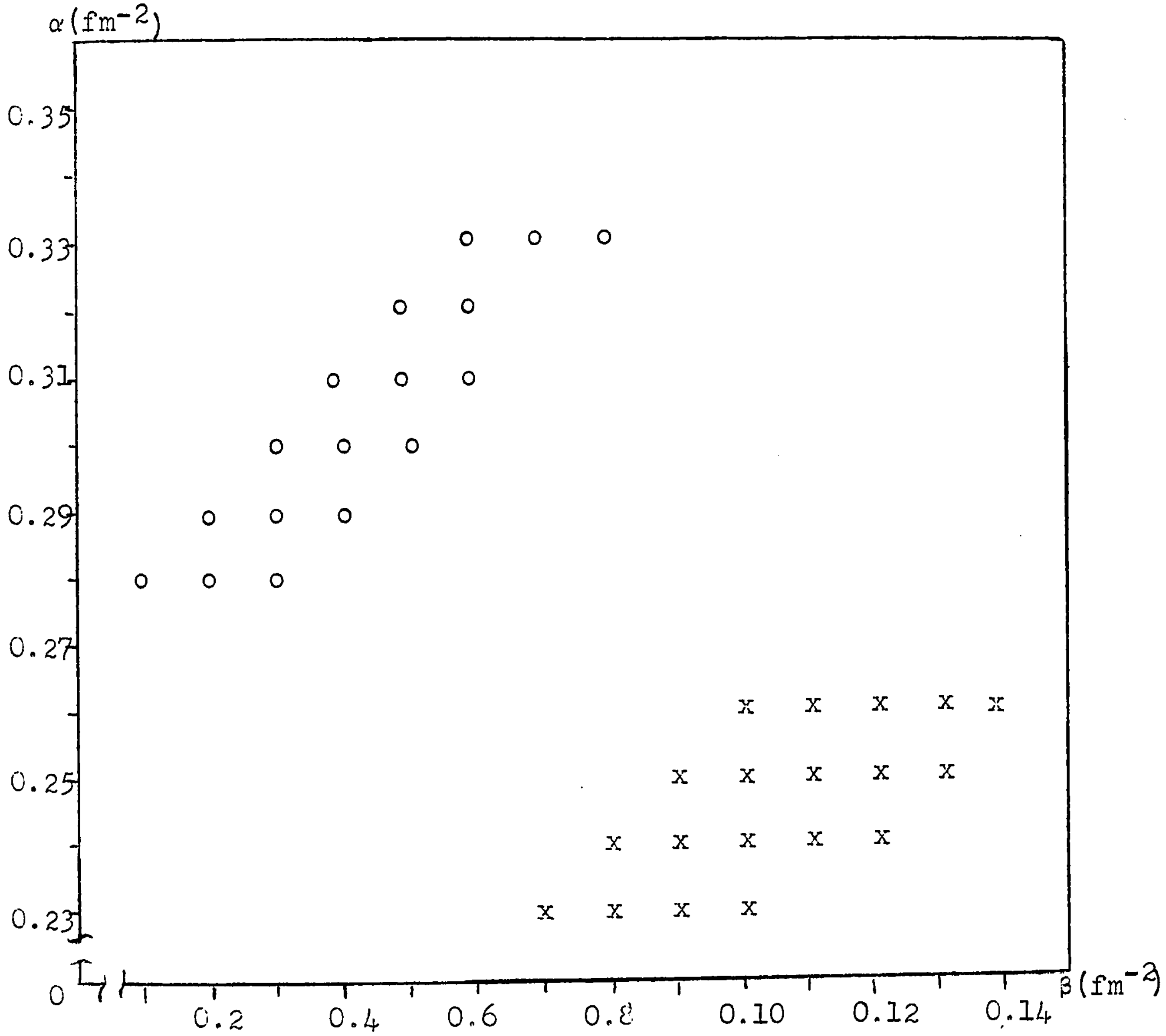


Fig. 12 Possible Cluster Model Parameter for the First Excited State. X refers to the Transition Probability Calculation and o to the Energy Calculation.

In the transition probability calculation, the operator is proportional to the sum of the $\vec{r}$'s of the protons only. Consequently, the greatest contribution to the expectation value occurs from large values of r. The wavefunction gives the correct transition probability for large β and small α.

Thus the two operators used tested the wavefunction in different regions and it proved impossible to find a set of parameters which gave acceptable values for both expectation values. One concludes that the cluster model wavefunction does not provide a good representation of the state. One reason for this is that the width of the state is large: about 4 MeV. (12). Thus it may be an over-simplification to describe the state as an alpha-cluster and a neutron. An admixture of cluster model wavefunctions might be used to describe this state, but the calculations involved would be extremely lengthy. It should be noted that since no minimum was found in the energy calculations, the parameters obtained are not physically meaningful.

CHAPTER 7

CONCLUSIONS

Two different types of calculations were attempted. In the first, the cluster model wavefunction for the $3/2^+$ and $3/2^-$ states were decomposed into sums of harmonic oscillator shell model wavefunctions. In the second calculation an attempt is made to fit a set of cluster model parameters to experimental data for $1/2^-$ state.

In several parts of the thesis, the calculations did not yield the results expected. The calculations related to the $3/2^-$ state indicate that the shell model constituents of the cluster model wavefunction describing the state have been largely determined. The majority of the shell model constituents for the $3/2^+$ state have not been found, and it is not evident what the most important constituents of this state are. The description of the $1/2^-$ state has again proved elusive.

In principle the constituents of the $3/2^+$ state could be determined by this method; however, it was indicated that this would be a very lengthy calculation. Perhaps the inclusion of a hard core in the potential would lead to a better result for the $1/2^-$ state.

The method of linear transformations used to evaluate the integrals has several advantages. It allows the integrals to be cast into an exact closed form. A larger class of integrals can be evaluated by this method, compared to Mellin and Laplace integral transforms (4). This method should be generally applicable in similar studies.

APPENDIX A

THE NORMALIZATION CONSTANT

A.1 THE GROUND STATE CLUSTER MODEL WAVEFUNCTION

The normalization constant is defined by [(1)]

$$N^2_{CM}\langle(1234;5)|(1234;5) - (5234;1)\rangle = 12 \tag{A-1}$$

where the spatial part of the wavefunction, denoted by (1234;5), was defined in eq. (2-1). It should be noted that this wavefunction as expressed in eq. (2-1) uses six non-independent variables. The first step is to express the wavefunction in terms of the five independent single-particle coordinates:

$$\begin{aligned}(1234;5) = \exp[-\{&P(r_1^2 + r_2^2 + r_3^2 + r_4^2) + Qr_5^2 \\ &+ R(\bar{r}_1.\bar{r}_2 + \bar{r}_1.\bar{r}_3 + \bar{r}_1.\bar{r}_4 + \bar{r}_2.\bar{r}_3 + \bar{r}_2.\bar{r}_4 + \bar{r}_3.\bar{r}_4) \\ &+ S(\bar{r}_1.\bar{r}_5 + \bar{r}_2.\bar{r}_5 + \bar{r}_3.\bar{r}_5 + \bar{r}_4.\bar{r}_5)\}]\ [\tfrac{1}{4}r_1Y_1^m(\Omega_1) \\ &+ \tfrac{1}{4}r_2Y_1^m(\Omega_2) + \tfrac{1}{4}r_3Y_1^m(\Omega_3) + \tfrac{1}{4}r_4Y_1^m(\Omega_4) - r_5Y_1^m(\Omega_5)]\end{aligned} \tag{A-2}$$

where
$$P = \frac{3}{8}\alpha_1 + \frac{\beta'}{40} + \frac{\mu}{10}$$
$$R = \frac{-\alpha_1}{4} + \frac{\beta'}{20} + \frac{\mu}{5}$$
$$Q = \frac{2}{5}\beta' + \frac{\mu}{10}$$
$$S = \frac{1}{5}(\mu - \beta')$$

The reason for beginning in single-particle coordinates is that this is the most convenient form in which to effect the exchanges required by antisymmetrization. Thus the single-particle representation of the one-particle exchange ground state cluster model wavefunction becomes

$$\begin{aligned}(5234;1) = \exp[-\{&P(r_2^2 + r_3^2 + r_4^2 + r_5^2) + Qr_1^2 \\ &+ R(\bar{r}_2\cdot\bar{r}_3 + \bar{r}_2\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5) + S(\bar{r}_1\cdot\bar{r}_2 \\ &+ \bar{r}_1\cdot\bar{r}_3 + \bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5)\}]\,[-r_1Y_1^m(\Omega_1) + \tfrac{1}{4}r_2Y_1^m(\Omega_2) \\ &+ \tfrac{1}{4}r_3Y_1^m(\Omega_3) + \tfrac{1}{4}r_4Y_1^m(\Omega_4) + \tfrac{1}{4}r_5Y_1^m(\Omega_5)]\end{aligned} \qquad (A\text{-}3)$$

The direct and exchange integrals must next be formulated and evaluated. For the direct term

$$\langle(1234;5)|(1234;5)\rangle = \int \exp[-\{2P(r_1^2 + r_2^2 + r_3^2 + r_4^2) \qquad (A\text{-}4)$$

(A-4) con't

$$+ 2Qr_5^{\,2} + 2R(\bar{r}_1\cdot\bar{r}_2 + \bar{r}_1\cdot\bar{r}_3 + \bar{r}_1\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_3 + \bar{r}_2\cdot\bar{r}_4$$

$$+ \bar{r}_3\cdot\bar{r}_4) + 2S(\bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_5 + \bar{r}_4\cdot\bar{r}_5)\}]\,|\tfrac{1}{4}r_1Y_1^m(\Omega_1)$$

$$+ \tfrac{1}{4}r_2Y_2^m(\Omega_2) + \tfrac{1}{4}r_3Y_1^m(\Omega_3) + \tfrac{1}{4}r_4Y_1^m(\Omega_4) - r_5Y_1^m(\Omega_5)|^2$$

$$d\bar{r}_1\ d\bar{r}_2\ d\bar{r}_3\ d\bar{r}_4\ d\bar{r}_5 \qquad \text{(A-4)}$$

The integrand can now be expressed in terms of variables obtained by taking linear combinations of the single-particle coordinates in such a manner that first, the polynomial part of an integrand contains the fewest number of terms, and second, the exponent contains no cross-terms. The polynomial part is simplified by a transformation which introduces the relative coordinate between the alpha-particle cluster and the neutron as one of the new variables:

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

$$\bar{\zeta}_2 = \bar{r}_1$$

$$\bar{\zeta}_3 = \bar{r}_2$$

$$\bar{\zeta}_4 = \bar{r}_4$$

$$\bar{\zeta}_5 = \bar{r}_5 \qquad \text{(A-5)}$$

Under this transformation the integral becomes

$$\begin{aligned}
\langle(1234;5)|(1234;5)\rangle = |J_1|^3 \int \exp\{-(&A(1)\zeta_1{}^2 + A(2)\bar{\zeta}_1\cdot\bar{\zeta}_2 \\
&+ A(3)\zeta_2{}^2 + A(4)\bar{\zeta}_1\cdot\bar{\zeta}_3 + A(5)\bar{\zeta}_2\cdot\bar{\zeta}_3 + A(6)\zeta_3{}^2 + A(7)\bar{\zeta}_1\cdot\bar{\zeta}_4 \\
&+ A(8)\bar{\zeta}_2\cdot\bar{\zeta}_4 + A(9)\bar{\zeta}_3\cdot\bar{\zeta}_4 + A(10)\zeta_4{}^2 + A(11)\bar{\zeta}_1\cdot\bar{\zeta}_5 \\
&+ A(12)\bar{\zeta}_2\cdot\bar{\zeta}_5 + A(13)\bar{\zeta}_3\cdot\bar{\zeta}_5 + A(14)\bar{\zeta}_4\cdot\bar{\zeta}_5 + A(15)\zeta_5{}^2)\} \\
&\zeta_1{}^2 Y_1^{m*}(\Omega_1) Y_1^m(\Omega_1)\, d\bar{\zeta}_1\, d\bar{\zeta}_2\, d\bar{\zeta}_3\, d\bar{\zeta}_4\, d\bar{\zeta}_5 \qquad \text{(A-6)}
\end{aligned}$$

where

$$\begin{aligned}
A(1) &= 16\left(\frac{\mu}{5} + \frac{3\alpha'}{4} + \frac{\beta'}{20}\right) \\
A(2) &= -8\alpha' \\
A(3) &= 2\alpha' \\
A(4) &= -8\alpha' \\
A(5) &= 2\alpha' \\
A(6) &= 2\alpha' \\
A(7) &= -8\alpha' \\
A(8) &= 2\alpha' \\
A(9) &= 2\alpha' \\
A(10) &= 2\alpha' \\
A(11) &= 8(\mu + 3\alpha') \\
A(12) &= -8\alpha' \\
A(13) &= -8\alpha'
\end{aligned}$$

$$A(14) = -8\alpha'$$

$$A(15) = 15\mu + 12\alpha'$$

$$J_1 = \frac{\partial(\bar{\zeta}_1, \bar{\zeta}_2, \bar{\zeta}_3, \bar{\zeta}_4, \bar{\zeta}_5)}{\partial(\bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4, \bar{r}_5)} = 4$$

The next step is to eliminate the scalar products in the exponent. The method used to generate this transformation is given in Appendix C. The transformation used is

$$\begin{aligned}
\bar{\zeta}_1 &= \bar{\xi}_1 \\
\bar{\zeta}_2 &= E(2)\bar{\xi}_1 + \bar{\xi}_2 \\
\bar{\zeta}_3 &= E(4)\bar{\xi}_1 + E(5)\bar{\xi}_2 + \bar{\xi}_3 \\
\bar{\zeta}_4 &= E(7)\bar{\xi}_1 + E(8)\bar{\xi}_2 + E(9)\bar{\xi}_3 + \bar{\xi}_4 \\
\bar{\zeta}_5 &= E(11)\bar{\xi}_1 + E(12)\bar{\zeta}_2 + E(13)\bar{\xi}_3 + E(14)\bar{\xi}_4 + \bar{\xi}_5
\end{aligned} \tag{A-7}$$

The Jacobian of this transformation is unity; so that under this transformation the integral becomes

$$\langle 1234;5) | (1234;5)\rangle = |J_1|^3 \int \exp\{-[\xi_1{}^2 E(1) + E(3)\xi_2{}^2 + E(6)\xi_3{}^2 + E(10)\xi_4{}^2 + E(15)\xi_5{}^2]\}\xi_1{}^2 Y_1^{m*}(\Omega_1) Y_1^m(\Omega_1) \, d\bar{\xi}_1 \, d\bar{\xi}_2 \, d\bar{\xi}_3 \, d\bar{\xi}_4 \, d\bar{\xi}_5 \tag{A-8}$$

The reason for introducing the relative motion coordinate should be now more apparent. There is only one term in the polynomial part of this last equation. If the relative coordinate had not been introduced, there would have been twenty-five; five of these would have remained after integrating over angles. In later cases the work saved by this type of transformation is considerable.

In terms of the transformation coefficients defined in Appendix C, the integral is

$$\langle (1234;5) | (1234;5) \rangle = \frac{24\pi^{13/2}}{E(1)\,[E(1)\ E(3)\ E(6)\ E(10)\ E(15)]^{3/2}} \tag{A-9}$$

The single-particle representation of the exchange integral is:

$$\begin{aligned}
\langle (1234;5) | (5234;1) \rangle = \int \exp\,[&-(P + Q)\,({r_1}^2 + {r_5}^2) \\
&- 2P({r_2}^2 + {r_3}^2 + {r_4}^2) - (R + S)\,(\bar{r}_1\cdot\bar{r}_2 + \bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_4 \\
&+ \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_5 + \bar{r}_4\cdot\bar{r}_5) - 2R(\bar{r}_2\cdot\bar{r}_3 + \bar{r}_2\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_4) \\
&- 2S\ \bar{r}_1\cdot\bar{r}_5]\{\tfrac{1}{4}r_1 Y_1^m(\Omega_1) + \tfrac{1}{4}r_2 Y_1^m(\Omega_2) + \tfrac{1}{4}r_3 Y_1^m(\Omega_3) \\
&+ \tfrac{1}{4}r_4 Y_1^m(\Omega_4) - r_5 Y_1^m(\Omega_5)\}\ \ \{-r_1 Y_1^{m*}(\Omega_1) + \tfrac{1}{4}r_2 Y_1^{m*}(\Omega_2) \\
&+ \tfrac{1}{3}r_3 Y_1^{m*}(\Omega_3) + \tfrac{1}{4}r_4 Y_1^{m*}(\Omega_4) + \tfrac{1}{4}r_5 Y_1^{m*}(\Omega_5)\} \\
&d\bar{r}_1\ d\bar{r}_2\ d\bar{r}_3\ d\bar{r}_4\ d\bar{r}_5
\end{aligned} \tag{A-10}$$

The following transformation is used to simplify the polynomial part of the integral

$$
\begin{aligned}
\bar{\zeta}_1 &= \frac{1}{4}\bar{r}_1 + \frac{1}{4}\bar{r}_2 + \frac{1}{4}\bar{r}_3 + \frac{1}{4}\bar{r}_4 - \bar{r}_5 \\
\bar{\zeta}_2 &= \bar{r}_2 \\
\bar{\zeta}_3 &= -\bar{r}_1 + \frac{1}{4}\bar{r}_2 + \frac{1}{4}\bar{r}_3 + \frac{1}{4}\bar{r}_4 + \frac{1}{4}\bar{r}_5 \\
\bar{\zeta}_4 &= \bar{r}_4 \\
\bar{\zeta}_5 &= \bar{r}_5
\end{aligned}
\qquad \text{(A-11)}
$$

where

$$
J = \frac{\partial(\bar{\zeta}_1, \bar{\zeta}_2, \bar{\zeta}_3, \bar{\zeta}_4, \bar{\zeta}_5)}{\partial(\bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4, \bar{r}_5)} = 3.2
$$

As the exchange integral is considered, there are two relative motions to be introduced. The exchange integral is transformed into

$$
\langle(1234;5)|(5234;1)\rangle = |J|^3 \int e^{-\varphi}\, \zeta_1 Y_1^{m*}(\Omega_1) \zeta_3 Y_1^{m}(\Omega_3)\, d\bar{\zeta}_1\, d\bar{\zeta}_2\, d\bar{\zeta}_3\, d\bar{\zeta}_4\, d\bar{\zeta}_5 \qquad \text{(A-12)}
$$

where φ has the same form as the exponent in eq. (A-6), except that the A's assume different values. Explicitly,

$$
\begin{aligned}
A(1) &= \frac{16}{25}\,(16V + W + 4Y) \\
A(2) &= -\frac{16}{25}\,(2V - X)
\end{aligned}
$$

$$A(3) = 2V - X)$$

$$A(4) = -\frac{16}{5}(2V - X)$$

$$A(5) = 2V - X$$

$$A(6) = 2V - X$$

$$A(7) = -\frac{8}{25}(4W - 16V + 6Y)$$

$$A(8) = -\frac{4}{5}(2V - X)$$

$$A(9) = 2V - X$$

$$A(10) = 2V - X$$

$$A(11) = -\frac{16}{5}(2V - X)$$

$$A(12) = 2V - X$$

$$A(13) = -\frac{4}{5}(2V - X)$$

$$A(14) = 2V - X$$

$$A(15) = 2V - X$$

$$V = \frac{3}{4}\alpha' + \frac{\beta'}{20} + \frac{\mu}{5}$$

$$W = \frac{3}{4}\alpha' + \frac{17}{40}\beta' + \frac{\mu}{5}$$

$$X = -\frac{\alpha'}{2} + \frac{\beta'}{10} + \frac{2\mu}{5}$$

$$Y = -\frac{\alpha'}{4} + \frac{3}{20}\beta' + \frac{2\mu}{5}$$

$$Z = \frac{2}{5}(\mu - \beta')$$

At this point, a transformation is used which changes the name of some of the variables. The result is that the integrand, after having its cross terms removed, has the minimal number of terms. The transformation used is

$$\begin{aligned} \bar{\xi}_1 &= \bar{\zeta}_1 \\ \bar{\xi}_2 &= \bar{\zeta}_3 \\ \bar{\xi}_3 &= \bar{\zeta}_2 \\ \bar{\xi}_4 &= \bar{\zeta}_4 \\ \bar{\xi}_5 &= \bar{\zeta}_5 \end{aligned} \tag{A-13}$$

Then eq. (A-12) becomes

$$\langle (1234;5) | (5234;1) \rangle = |J|^3 \int e^{-\varphi} \xi_1 Y_1^{m*}(\Omega_1) \xi_2 Y_1^m(\Omega_2) \, d\bar{\xi}_1 \, d\bar{\xi}_2 \, d\bar{\xi}_3 \, d\bar{\xi}_4 \, d\bar{\xi}_5 \tag{A-14}$$

When the cross terms are removed from eq. (A-14) using a transformation similar to eq. (A-7), the integral becomes

$$\langle (1234;5) | (5234;1) \rangle = |J|^3 \int \exp \{ -E(1)\rho_1{}^2 - E(3)\rho_2{}^2 - E(6)\rho_3{}^2 - E(10)\rho_4{}^2 - E(15)\rho_5{}^2 \} \rho_1 Y_1^{m*}(\Omega_1) [E(2)\rho_1 Y_1^m(\Omega_1) + \rho_2 Y_1^m(\Omega_2)] \, d\bar{\rho}_1 \, d\bar{\rho}_2 \, d\bar{\rho}_3 \, d\bar{\rho}_4 \, d\bar{\rho}_5 \tag{A-15}$$

This may be evaluated explicitly, yielding,

$$\langle (1234;5) | (5234;1) \rangle = \frac{3\pi^{13/2} (3.2)^3 \, E(2)}{8E(1) \, [E(1) \, E(3) \, E(6) \, E(10) \, E(15)]^{3/2}} \qquad \text{(A-16)}$$

where the E's are defined in Appendix C.

Thus, for the ground state, the cluster model wavefunction normalization constant is

$$N_{CM}{}^2 = \frac{12}{\langle (1234;5) | (1234;5) \rangle - \langle (1234;5) | (5234;1) \rangle} \qquad \text{(A-17)}$$

A.2 SINGLE-PARTICLE WAVEFUNCTION FOR THE GROUND STATE

Since the spin part of the single-particle wavefunction is the same as that of the cluster model wavefunction, eq. (A-1) can be used as the definition of the normalization constants for these states as well.

In this case the calculation of the normalization constant is not as involved as for the cluster model, because the exponent written in terms of the single-particle coordinates contains no cross terms (i.e. terms of the form $\bar{r}_1 \cdot \bar{r}_2$).

The exchange integral will be considered first.

If nucleons 1 and 5 are in different states, (as is always the case), the orthogonality of the harmonic oscillator wavefunctions yields:

$$\langle (12345) | (52341) \rangle = 0. \qquad \text{(A-18)}$$

The direct terms were evaluated using eq. (7-148) of Powell and Crasemann (13). The resulting integrals appear in Table 5.

A.3 THE SECOND EXCITED STATE CLUSTER MODEL WAVEFUNCTION

The calculation of the normalization constant for the second excited state is different from that of the ground state in detail but not in principle. The definition of the normalization constant is (1)

$$N_{CM}^2 \langle (123;45) | (123;45) - 2(124;35) + (524;31) \rangle = 8 \qquad \text{(A-19)}$$

The single-particle representation of the cluster model wavefunction (3-1) is

$$(123;45) = \exp [-\{P(r_1^2 + r_2^2 + r_3^2) + Q(r_4^2 + r_5^2$$

$$+ R(\bar{r}_1 \cdot \bar{r}_2 + \bar{r}_1 \cdot \bar{r}_3 + \bar{r}_2 \cdot \bar{r}_3) + S(\bar{r}_1 \cdot \bar{r}_4 + \bar{r}_1 \cdot \bar{r}_5 + \bar{r}_2 \cdot \bar{r}_4 \qquad \text{(A-20)}$$

TABLE 5

NORMALIZATION CONSTANTS FOR THE SHELL MODEL WAVEFUNCTIONS WHICH CONTRIBUTE TO THE $3/2^-$ CLUSTER MODEL WAVEFUNCTION

CONFIGURATION	DIRECT INTEGRAL
$(1s)^4(1p)$	$\frac{3\pi^{13/2}}{8\mu^{17/2}}$
$(1s)^3(1p)(2s)$	$\frac{9\pi^{13/2}}{16\mu^{17/2}}$
$(1s)^4(2p)$	$\frac{15\pi^{13/2}}{16\mu^{17/2}}$
$(1s)^4(3p)$	$\frac{105\pi^{13/2}}{64\mu^{17/2}}$

(A-20) con't

$$+ \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5) + T\bar{r}_4\cdot\bar{r}_5\}] \{\frac{1}{9} (r_1^2 + r_2^2 + r_3^2$$

$$+ 2\bar{r}_1\cdot\bar{r}_2 + 2\bar{r}_1\cdot\bar{r}_3 + 2\bar{r}_2\cdot\bar{r}_3) + \frac{1}{4}[r_4^2 + r_5^2 + 2\bar{r}_4\cdot\bar{r}_5]$$

$$- \frac{1}{3}[\bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5]\}$$

where

$$P = \frac{\alpha}{3} + \frac{\beta}{15} + \frac{\mu}{10}$$

$$Q = \frac{\alpha}{4} + \frac{3}{20}\beta + \frac{\mu}{10}$$

$$R = -\frac{1}{3}\alpha + \frac{2}{15}\beta + \frac{\mu}{5}$$

$$S = \frac{1}{5}(\mu - \beta)$$

$$T = \frac{\alpha}{2} + \frac{3\beta}{10} + \frac{\mu}{5}$$

The single-particle representation of the one-particle and two-particle exchange wavefunction is

$$(124;35) = \exp[-\{P(r_1^2 + r_2^2 + r_4^2) + Q(r_3^2 + r_5^2)$$

$$+ R(\bar{r}_1\cdot\bar{r}_2 + \bar{r}_1\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_4) + S(\bar{r}_1\cdot\bar{r}_3 + \bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_3$$

$$+ \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_4\cdot\bar{r}_5] + T\bar{r}_3\cdot\bar{r}_5\}] \{\frac{1}{9} (r_1^2 + r_2^2 + r_3^2$$

$$+ 2\bar{r}_1\cdot\bar{r}_2 + 2\bar{r}_1\cdot\bar{r}_4 + 2\bar{r}_2\cdot\bar{r}_4) + \frac{1}{4} (r_3^2 + r_5^2 + 2\bar{r}_2\cdot\bar{r}_5$$

$$- \frac{1}{3} (\bar{r}_1\cdot\bar{r}_3 + \bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_3 + \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_4\cdot\bar{r}_5)\}$$

(A-21)

and:

$$\begin{aligned}
(524;31) = \exp - \{&P(r_2^2 + r_4^2 + r_5^2) + Q(r_1^2 + r_3^2) \\
&+ R(\bar{r}_2\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_5 + \bar{r}_4\cdot\bar{r}_5) + S(\bar{r}_1\cdot\bar{r}_2 + \bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5 \\
&+ \bar{r}_2\cdot\bar{r}_3 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5) + T\bar{r}_1\cdot\bar{r}_3\} [\tfrac{1}{9}(r_2^2 + r_4^3 + r_5^2 \\
&+ 2\bar{r}_2\cdot\bar{r}_4 + 2\bar{r}_2\cdot\bar{r}_5 + 2\bar{r}_4\cdot\bar{r}_5) + \tfrac{1}{4}(r_1^2 + r_3^2 + 2\bar{r}_1\cdot\bar{r}_3) \\
&- \tfrac{1}{3}(\bar{r}_1\cdot\bar{r}_2 + \bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_3 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5)]
\end{aligned} \tag{A-22}$$

respectively. In these cases, there are three integrals to be evaluated: the direct, one- and two-particle exchange terms. The direct term may be represented as

$$\begin{aligned}
\langle(123;45)|(123;45)\rangle = \int \exp - \{&2P(r_1^2 + r_2^2 + r_3^2) \\
&+ 2Q(r_4^2 + r_5^2) + 2R(\bar{r}_1\cdot\bar{r}_2 + \bar{r}_1\cdot\bar{r}_3 + \bar{r}_2\cdot\bar{r}_3) + 2S(\bar{r}_1\cdot\bar{r}_4 \\
&+ \bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_5) + T(\bar{r}_4\cdot\bar{r}_5)\}\{\tfrac{1}{9}(r_1^2 \\
&+ r_2^2 + r_3^2 + 2\bar{r}_1\cdot\bar{r}_2 + 2\bar{r}_1\cdot\bar{r}_3 + 2\bar{r}_2\cdot\bar{r}_3) + \tfrac{1}{4}(r_4^2 \\
&+ r_5^2 + 2r_4\cdot r_5) - \tfrac{1}{3}(\bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_5 \\
&+ \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5)\}^2 \, d\bar{r}_1 \, d\bar{r}_2 \, d\bar{r}_3 \, d\bar{r}_4 \, d\bar{r}_5
\end{aligned} \tag{A-23}$$

The first transformation used introduces the relative coordinate. This is useful in reducing the number of terms in the polynomial part of the integrand. The transformation is

$$\begin{aligned}
\bar{\xi}_1 &= \frac{1}{3}(\bar{r}_1 + \bar{r}_2 + \bar{r}_3) - \frac{1}{2}(\bar{r}_4 + \bar{r}_5) \\
\bar{\xi}_2 &= \bar{r}_2 \\
\bar{\xi}_3 &= \bar{r}_3 \\
\bar{\xi}_4 &= \bar{r}_4 \\
\bar{\xi}_5 &= \bar{r}_5
\end{aligned} \tag{A-24}$$

The Jacobian of this transformation is

$$J = \frac{\partial(\bar{\xi}_1, \bar{\xi}_2, \bar{\xi}_3, \bar{\xi}_4, \bar{\xi}_5)}{\partial(\bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4, \bar{r}_5)} = \frac{1}{3}$$

Thus, the integral is eq. (A-23) becomes

$$\langle(123;45)|(123;45)\rangle \; |J|^3 \int e^{-\varphi} \, \xi_1^4 \; d\bar{\xi}_1 \, d\bar{\xi}_2 \, d\bar{\xi}_3 \, d\bar{\xi}_4 \, d\bar{\xi}_5 \tag{A-25}$$

where φ is the same exponent as in eq. (A-6) with different values for the A's. Explicitly,

$$A(1) = 18P$$

$$A(2) = -6(2P - R)$$

$$A(3) = 2(2P - R)$$

$$A(4) = -6(2P - R)$$

$$A(5) = 2(2P - R)$$

$$A(6) = 2(2P - R)$$

$$A(7) = 6(3P + S)$$

$$A(8) = -3(2P - R)$$

$$A(9) = -3(2P - R)$$

$$A(10) = 2Q + \frac{9}{2} P + 3S$$

$$A(11) = 6(3P + S)$$

$$A(12) = -3(2P - R)$$

$$A(13) = -3(2P - R)$$

$$A(14) = 2T + 9P + 6S$$

$$A(15) = 2Q + \frac{9}{2}P + 3S$$

By applying the transformation similar to that in eq. (A-7), the cross-terms in the exponent are eliminated and the integral becomes

$$\langle (123;45) | (123;45) \rangle = |J|^3 \int \exp -\{E(1)\rho_1{}^2 + E(3)\rho_2{}^2 + E(6)\rho_3{}^2 + E(10)\rho_4{}^2 + E(15)\rho_5{}^2\} \, \rho_1{}^4 \, d\bar{\rho}_1 \, d\bar{\rho}_2 \, d\bar{\rho}_3 \, d\bar{\rho}_4 \, d\bar{\rho}_5 \qquad \text{(A-26)}$$

This can be reduced to the form

$$\langle(123;45)|(123;45)\rangle = \frac{405\pi^{15/2}}{4(E(1))^2[E(1)\ E(3)\ E(6)\ E(10)\ E(15)]^{3/2}}$$

(A-27)

The single-particle representation of the one-particle exchange integral is

$$\langle(123;45)|(124;35)\rangle = \int \exp -\{2P[r_1^{\,2} + r_2^{\,2}] + (P + Q)(r_3^{\,2} + r_4^{\,2})$$

$$+ 2Qr_5^{\,2} + 2R\bar{r}_1\cdot\bar{r}_2 + (R + S)(\bar{r}_1\cdot\bar{r}_3 + \bar{r}_1\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_3 + \bar{r}_2\cdot\bar{r}_4)$$

$$+ 2S(\bar{r}_1\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_5) + (T + S)(\bar{r}_3\cdot\bar{r}_5 + \bar{r}_4\cdot\bar{r}_5)\}$$

$$\{\tfrac{1}{9}\,(r^{\,2} + r_2^{\,2} + r_3^{\,2} + 2\bar{r}_1\cdot\bar{r}_2 + 2\bar{r}_1\cdot\bar{r}_3 + 2\bar{r}_2\cdot\bar{r}_3)$$

$$+ \tfrac{1}{4}(r_4^{\,2} + r_5^{\,2} + 2\bar{r}_4\cdot\bar{r}_5) - \tfrac{1}{3}(\bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_4 + \bar{r}_2\cdot\bar{r}_5$$

$$+ \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5)\}\{\tfrac{1}{9}(r_1^{\,2} + r_2^{\,2} + r_3^{\,2} + 2r_1\cdot r_2 + 2r_1\cdot r_4$$

$$+ 2r_2\cdot r_4) + \tfrac{1}{4}(r_3^{\,2} + r_5^{\,2} + 2\bar{r}_2\cdot\bar{r}_5) - \tfrac{1}{3}(\bar{r}_1\cdot\bar{r}_3 + \bar{r}_1\cdot\bar{r}_5$$

$$\bar{r}_2\cdot\bar{r}_3 + \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_4\cdot\bar{r}_5)\}\ d\bar{r}_1\ d\bar{r}_2\ d\bar{r}_3\ d\bar{r}_4\ d\bar{r}_5$$

(A-28)

The polynomial part of the integral is simplified by introducing the relative coordinates, using the transformation

(A-29)

$$\bar{\xi}_1 = \bar{r}_1$$

(A-29) con't

$$\bar{\xi}_2 = \frac{1}{3}\bar{r}_1 + \frac{1}{3}\bar{r}_2 + \frac{1}{3}\bar{r}_3 - \frac{1}{2}\bar{r}_4 - \frac{1}{2}\bar{r}_5$$

$$\bar{\xi}_3 = \frac{1}{3}\bar{r}_1 + \frac{1}{3}\bar{r}_2 - \frac{1}{2}\bar{r}_3 + \frac{1}{3}\bar{r}_4 - \frac{1}{2}\bar{r}_5$$

$$\bar{\xi}_4 = \bar{r}_4$$

$$\bar{\xi}_5 = \bar{r}_5$$

Under this transformation eq. (A-28) becomes:

$$\langle(123;45)|(124.35)\rangle = |J|^3 \int \exp(-\varphi)\xi_2^2\,\xi_3^2 \, d\bar{\xi}_1\, d\bar{\xi}_2\, d\bar{\xi}_3\, d\bar{\xi}_4\, d\bar{\xi}_5 \qquad \text{(A-30)}$$

where

$$\varphi = B(1,1)\xi_1^2 + B(1,2)\bar{\xi}_1\cdot\bar{\xi}_2 + B(1,3)\bar{\xi}_2^2 + B(1,4)\bar{\xi}_1\cdot\bar{\xi}_3 + B(1,5)\bar{\xi}_2\cdot\bar{\xi}_3 + B(1,6)\xi_3^2 + B(1,7)\bar{\xi}_1\cdot\bar{\xi}_4 + B(1,8)\bar{\xi}_2\cdot\bar{\xi}_4 + B(1,9)\bar{\xi}_3\cdot\bar{\xi}_4 + B(1,10)\xi_4^2 + B(1,11)\bar{\xi}_1\cdot\bar{\xi}_5 + B(1,12)\bar{\xi}_2\cdot\bar{\xi}_5 + B(1,13)\bar{\xi}_3\cdot\bar{\xi}_5 + B(1,14)\bar{\xi}_4\cdot\bar{\xi}_5 + B(1,15)\xi_5^2 \qquad \text{(A-31)}$$

$$B(1,1) = 4P - 2R$$

$$B(1,2) = \frac{12}{5}(R - 2P)$$

$$B(1,3) = \frac{36}{25}(3P - R - S + Q)$$

$$B(1,4) = \frac{18}{5}(R - 2P)$$

$$B(1,5) = \frac{18}{25}(8P - R - S - 4Q)$$

$$B(1,6) = \frac{18}{5}(11P + 3R + 3S + 2Q)$$

$$B(1,7) = 2P - R$$

$$B(1,8) = \frac{3}{5}(3R - S - 4Q)$$

$$B(1,9) = \frac{3}{5}(10P + 7R + 11S + 4Q)$$

$$B(1,10) = \frac{5P}{2} + 2Q + R + 3S$$

$$B(1,11) = -6P + 3R$$

$$B(1,12) = \frac{3}{5}(12P - 3R - S - 2T)$$

$$B(1,13) = \frac{3}{5}(18P + 3R + 2T + 11S)$$

$$B(1,14) = 3P + 2T + 6S + 3R$$

$$B(1,15) = 2Q + \frac{9}{2}P + 3S$$

$$J = \frac{\partial(\bar{\rho}_1, \bar{\rho}_2, \bar{\rho}_3, \bar{\rho}_4, \bar{\rho}_5)}{\partial(\bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4, \bar{r}_5)} = 3.6$$

It will be noted that in this case the coefficients from the exponent are double subscripted variables. It will be shown that the two-particle exchange integral can be expressed in the form of eq. (A-30). The final form of the one- and two-particle exchange integral will be identical to that of the other, thus reducing the amount of work required. Although these integrals can be expressed in the same form the value of the B's will change between the two integrals. The additional index identifies the integral described.

To elucidate further, the single-particle representation of the two-particle exchange integral is

$$\begin{aligned}
&\langle(123;45)|(524;31)\rangle = \int \exp - \{2Pr_2^2 + (P + Q)(r_1^2 \\
&+ r_3^2 + r_4^2 + r_5^2) + (R + S)(\bar{r}_1\cdot\bar{r}_2\cdot + \bar{r}_2\cdot\bar{r}_3 + \bar{r}_2\cdot\bar{r}_4 \\
&+ \bar{r}_2\cdot\bar{r}_5) + 2S(\bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5) + (T + S) \\
&(\bar{r}_1\cdot\bar{r}_3 + \bar{r}_4\cdot\bar{r}_5)\} \{\tfrac{1}{9} (r_1^2 + r_2^2 + r_3^2 + 2r_1\cdot r_2 + 2r_1\cdot r_3 \\
&+ 2\bar{r}_2\cdot\bar{r}_5) + \tfrac{1}{4} (r_4^2 + r_5^2 + 2r_4\cdot r_5) - \tfrac{1}{3} (\bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5 \\
&+ \bar{r}_2\cdot\bar{r}_5 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5)\} \{\tfrac{1}{9} (r_2^2 + r_4^2 + r_5^2 + 2\bar{r}_2\cdot\bar{r}_4 \\
&+ 2\bar{r}_2\cdot\bar{r}_5 + 2\bar{r}_4\cdot\bar{r}_5) + \tfrac{1}{4}(r_1^2 + r_3^2 + 2\bar{r}_1\cdot\bar{r}_3) - \tfrac{1}{3}(\bar{r}_1\cdot\bar{r}_2 \\
&+ \bar{r}_1\cdot\bar{r}_4 + \bar{r}_1\cdot\bar{r}_5 + \bar{r}_2\cdot\bar{r}_3 + \bar{r}_3\cdot\bar{r}_4 + \bar{r}_3\cdot\bar{r}_5)\} \\
&d\bar{r}_1\, d\bar{r}_2\, d\bar{r}_3\, d\bar{r}_4\, d\bar{r}_5 \qquad \text{(A-31)}
\end{aligned}$$

In this case the transformation used to introduce the relative coordinates is:

$$\bar{\xi}_1 = \bar{r}_1$$

$$\bar{\xi}_2 = \frac{1}{3}\bar{r}_1 + \frac{1}{3}\bar{r}_2 + \frac{1}{3}\bar{r}_3 - \frac{1}{2}\bar{r}_4 - \frac{1}{2}\bar{r}_5$$

$$\bar{\xi}_3 = -\frac{1}{2}\bar{r}_1 + \frac{1}{3}\bar{r}_2 - \frac{1}{2}\bar{r}_3 + \frac{1}{3}\bar{r}_4 + \frac{1}{3}\bar{r}_5$$

$$\bar{\xi}_4 = \bar{r}_4$$

$$\bar{\xi}_5 = \bar{r}_5 \tag{A-32}$$

As previously stated, under this transformation eq. (A-31) becomes (A-30), where

$$\varphi = B(2,1)\xi_1^2 + B(2,2)\bar{\xi}_1\cdot\bar{\xi}_2 + B(2,3)\xi_2^2 + B(2,4)\bar{\xi}_1\cdot\bar{\xi}_3$$
$$+ B(2,5)\bar{\xi}_2\cdot\bar{\xi}_3 + B(2,6)\xi_3^2 + B(2,7)\bar{\xi}_1\cdot\bar{\xi}_4 + B(2,8)\bar{\xi}_2\cdot\bar{\xi}_4$$
$$+ B(2,9)\bar{\xi}_3\cdot\bar{\xi}_4 + B(2,10)\xi_4^2 + B(2,11)\bar{\xi}_1\cdot\bar{\xi}_5 + B(2,12)\bar{\xi}_2\cdot\bar{\xi}_5$$
$$+ B(2,13)\bar{\xi}_3\cdot\bar{\xi}_5 + B(2,14)\bar{\xi}_4\cdot\bar{\xi}_5 + B(2,15)\xi_5^2$$

$$B(2,1) = \frac{5}{2}P + 2Q + R + 3S$$

$$B(2,2) = \frac{3}{5}(3R - 4Q - S)$$

$$B(2,3) = \frac{36}{25}(3P + Q - R - S)$$

$$B(2,4) = \frac{3}{5}(10P + 7R + 11S + 4Q)$$

$$B(2,5) = \frac{18}{25}(8P - R - S - 4Q)$$

$$B(2.6) = \frac{18}{25}(11P + 3R + 3S + 2Q)$$

$$B(2,7) = 3P + 2Q + 3R + T + 6S$$

$$B(2,8) = \frac{3}{5}(-4Q + 3R - S)$$

$$B(2,9) = \frac{3}{5}(10P + 7R + 11S + 4Q)$$

$$B(2,10) = \frac{5}{2}P + 2Q + 6R + 3S$$

$$B(2,11) = T + R - 2P - 2Q$$

$$B(2,12) = \frac{6}{5}(2P + 2Q - T - R)$$

$$B(2,13) = -\frac{6}{5}(2P + 2Q - T - R)$$

$$B(2,14) = T + R - 2P - 2Q$$

$$B(2,15) = -T - R + 2P + 2Q$$

$$J = \frac{\partial(\bar{\xi}_1, \bar{\xi}_2, \bar{\xi}_3, \bar{\xi}_4, \bar{\xi}_5)}{\partial(r_1, r_2, r_3, r_4, r_5)} = 3.6$$

The next transformation is used as a matter of convenience so that when the transformation which removes the cross terms in the exponent is applied there is a minimum number of terms in the polynomial part. The transformation used is

$$\begin{aligned} \bar{\rho}_1 &= \bar{\xi}_2 \\ \bar{\rho}_2 &= \bar{\xi}_3 \\ \bar{\rho}_3 &= \bar{\xi}_1 \\ \bar{\rho}_4 &= \bar{\xi}_4 \\ \bar{\rho}_5 &= \bar{\xi}_5 \end{aligned} \qquad \text{(A-33)}$$

$$\langle(123;45)|(124.35) = |J|^3 \int \exp(-\varphi)\rho_1^2\rho_2^2$$

$$d\bar{\rho}_1\, d\bar{\rho}_2\, d\bar{\rho}_3\, d\bar{\rho}_4\, d\bar{\rho}_5 \qquad \text{(A-34)}$$

Then eq. (A-30) assumes the same form as eq. (A-34), and is defined in eq. (A-6). The A's are defined as follows, where k = 1 indicates a one-particle exchange, and k = 2 indicates a two-particle exchange.

$A(1) = B(k,3)$

$A(2) = B(k,5)$

$A(3) = B(k,6)$

$A(4) = B(k,2)$

$A(5) = B(k,4)$

$A(6) = B(k,1)$

$A(7) = B(k,8)$

$A(8) = B(k,9)$

$A(9) = B(k,7)$

$A(10) = B(k,10)$

$A(11) = B(k,13)$

$A(12) = B(k,11)$

$A(13) = B(k,12)$

$A(14) = B(k,14)$

$A(15) = B(k,15)$

After applying eq. (A-7) and performing some alegbra, eq. (A-30) assumes the form

$$\frac{3 \times 3.6^3 \pi^{15/2}}{4E(1)[E(1)\ E(3)\ E(6)\ E(10)\ E(15)]^{3/2}} \left[\frac{3}{E(3)} + \frac{5\ E(2)^2}{E(1)} \right] \tag{A-35}$$

Thus the normalization constant for the second excited state cluster model wavefunction can be found.

A.4 SINGLE-PARTICLE WAVEFUNCTIONS FOR THE SECOND EXCITED STATE

The spin part of single-particle wavefunctions is of the same form as that of the cluster model wavefunctions; consequently, eq. (A-10) is also the definition of the shell model normalization constant. Since the exchange terms are created by exchanging nucleons in different states, it follows from orthogonality that the exchange integrals are zero. The different integrals were determined using eq. (7-148) of Powell anc Crasemann,(13) and are given in Table 6.

TABLE 6

NORMALIZATION CONSTANT FOR THE SHELL MODEL WAVEFUNCTIONS WHICH CONTRIBUTE TO THE $3/2^+$ CLUSTER MODEL WAVEFUNCTION

CONFIGURATION	DIRECT INTEGRAL
$(1s)^3(1p)^2$	$\frac{3\pi^{13/2}}{8\mu^{17/2}}$
$(1s)^2(1p)(2s)$	$\frac{9\pi^{13/2}}{16\mu^{17/2}}$
$(1s)^3(1p)(2p)$	$\frac{15\pi^{13/2}}{16\mu^{17/2}}$
$(1s)^3(2p)^2$	$\frac{15\pi^{13/2}}{16\mu^{17/2}}$

APPENDIX B

THE OVERLAP INTEGRAL

B.1 THE GROUND STATE

For each shell model configuration used in the expansion of the ground state wavefunction, there are two overlap integrals to be evaluated, the direct term and the exchange term. The approach which has been followed is to transform each integral in such a way that both assume the same form, so that there is only one closed form per configuration.

To illustrate this procedure, consider the direct integral of eq. (2-6) first. The first transformation is used to reduce the number of terms in the polynomial part of the integrand. This is accomplished by

$$\begin{aligned}
\bar{\zeta}_1 &= \bar{r}_1 \\
\bar{\zeta}_2 &= \bar{r}_2 \\
\bar{\zeta}_3 &= \tfrac{1}{4}\bar{r}_1 + \tfrac{1}{4}\bar{r}_2 + \tfrac{1}{4}\bar{r}_3 + \tfrac{1}{4}\bar{r}_4 - \bar{r}_5 \\
\bar{\zeta}_4 &= \bar{r}_4 \\
\bar{\zeta}_5 &= \bar{r}_5
\end{aligned} \qquad \text{(B-1)}$$

Under this transformation, eq. (2-6) becomes

$$\langle (12334) | (1234;5) \rangle = J^3 \int e^{-\varphi_1} \xi_5 Y_1^{m*}(\Omega_5) \xi_3 Y_1^{m}(\Omega_3)$$

$$d\bar{\xi}_1 \, d\bar{\xi}_2 \, d\bar{\xi}_3 \, d\bar{\xi}_4 \, d\bar{\xi}_5 \qquad \text{(B-2)}$$

where

$$\varphi_1 = B(1,1)\xi_1^2 + B(1,2)\bar{\xi}_1 \cdot \bar{\xi}_2 + B(1,3)\xi_2^2 + B(1,4)\bar{\xi}_1 \cdot \bar{\xi}_3$$

$$+ B(1,5)\bar{\xi}_2 \cdot \bar{\xi}_3 + B(1,6)\xi_3^2 + B(1,7)\bar{\xi}_1 \cdot \bar{\xi}_4 + B(1,8)\bar{\xi}_2 \cdot \bar{\xi}_4$$

$$+ B(1,9)\bar{\xi}_2 \cdot \bar{\xi}_4 + B(1,10)\bar{\xi}_4^2 + B(1,11)\bar{\xi}_1 \cdot \bar{\xi}_5 + B(1,12)\bar{\xi}_2 \cdot \bar{\xi}_5$$

$$+ B(1,13)\bar{\xi}_3 \cdot \bar{\xi}_5 + B(1,14)\bar{\xi}_4 \cdot \bar{\xi}_5 + B(1,15)\xi_5^2$$

$B(1,1) = 2V - X$

$B(1,2) = 2V - X$

$B(1,3) = 2V - X$

$B(1,4) = -8V + 4X$

$B(1,5) = -8V + 4X$

$B(1,6) = 16V$

$B(1,7) = 2V - X$

$B(1,8) = 2V - X$

$B(1,9) = -8V + 4X$

$B(1,10) = 2V - X$

$$B(1,11) = -8V + 4X$$

$$B(1,12) = -8V + 4X$$

$$B(1,13) = -32V + 4Z$$

$$B(1,14) = -8V + 4X$$

$$B(1,15) = 16V + W + 4Z$$

$$V = \frac{3}{5}\mu + \frac{3}{8}\alpha' + \frac{\beta'}{40}$$

$$W = \frac{3}{5}\mu + \frac{2\beta'}{5}$$

$$X = \frac{\alpha'}{4} + \frac{\beta'}{20} + \frac{\mu}{5}$$

$$Z = \frac{1}{5}(\mu - \beta)$$

$$J = \frac{\partial(\bar{\xi}_1, \bar{\xi}_2, \bar{\xi}_3, \bar{\xi}_4, \bar{\xi}_5)}{\partial(\bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4, \bar{r}_5)} = \frac{1}{4}$$

It was stated at the beginning of this section that the direct and exchange integral will be transformed into the same integral. Thus, the additional subscript in the coefficients in the exponent is used to indicate which of the integrals is being considered.

The exchange integral eq. (2-7) is next transformed into eq. (B-2). This is accomplished by the transformation

$$\bar{\xi}_1 = \bar{r}_1$$

$$\bar{\xi}_2 = \bar{r}_2$$

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

$$\bar{\xi}_4 = \bar{r}_4$$

$$\bar{\xi}_5 = \bar{r}_5 \qquad \text{(B-3)}$$

In this case,

$$\varphi = B(2,1)\xi_1^2 + B92,2)\bar{\xi}_1 \cdot \bar{\xi}_2 + B(2,3)\xi_2^2 + B(2,4)\bar{\xi}_1 \cdot \bar{\xi}_3$$

$$+ B(2,5)\bar{\xi}_2 \cdot \bar{\xi}_3 + B(2,6)\xi_3^2 + B(2,7)\bar{\xi}_1 \cdot \bar{\xi}_4 + B(2,8)\bar{\xi}_2 \cdot \bar{\xi}_4)$$

$$+ B(2,9)\bar{\xi}_3 \cdot \bar{\xi}_4 + B(2,10)\bar{\xi}_4^2 + B(2,11)\bar{\xi}_1 \cdot \bar{\xi}_5 + B(2,13)\bar{\xi}_3 \cdot \bar{\xi}_5$$

$$+ B(2,14)\bar{\xi}_4 \cdot \bar{\xi}_5 + B(2,15)\xi_5^2$$

where

$B(2,1) = 16V + W + 4Z$

$B(2,2) = -8V + 4X$

$B(2,3) = 2V - X$

$B(2,4) = 32V + 4Z$

$B(2,5) = -8V + 4X$

$B(2,6) = 16V$

$B(2,7) = -8V + 4X$

$B(2,8) = 2V - X$

$B(2,9) = -8V + 4X$

$B(2,10) = 2V - X$

$B(2,11) = -8V + 4X$

$B(2,12) = 2V - X$

$B(2,13) = -8V + 4X$

$B(2,14) = 2V - X$

$B(2,15) = 2V - X$

It is possible to express all direct and exchange integrals, regardless of which configuration is considered, in a form in which the exponentials are the same as that in eq. (B-2). The polynomial part of the integrals will be different, but the exponents will all be the same. Thus the transformation applied to eq. (B-2) will depend on which configuration is being considered, i.e. depend on which variables are involved in the polynomial part.

The next transformation applied to eq. (B-2) simply redefines the variables in such a way that the most complicated variable in the polynomial part of this equation is called ρ_1, the next most complicated ρ_2, and so on. The motivation is this: when the transformation which removes the cross terms from the exponent is applied, the polynomial part of the integrand has the minimum number of terms. It is noted that this renaming transformation is neither unique nor necessary, but it makes the evaluation of the integral simpler.

As an example, the renaming transformation used for the configuration $(1s)^4(1p)$ is

$$\begin{aligned} \bar{\rho}_1 &= \bar{\xi}_3 \\ \bar{\rho}_2 &= \bar{\xi}_5 \\ \bar{\rho}_3 &= \bar{\xi}_1 \\ \bar{\rho}_4 &= \bar{\xi}_2 \\ \bar{\rho}_5 &= \bar{\xi}_4 \end{aligned} \qquad \text{(B-4)}$$

Under this transformation eq. (B-2) becomes

$$\langle (12345)_1 | (1234;5) \rangle = |J|^3 \int e^{-\varphi} \rho_1 Y_1^{m*}(\Omega_1) \rho_2 Y_1^m(\Omega_2)$$
$$d\bar{\rho}_1 \; d\bar{\rho}_2 \; d\bar{\rho}_3 \; d\bar{\rho}_4 \; d\bar{\rho}_5 \qquad \text{(B-5)}$$

where

$$\varphi \; A(1)\rho_1{}^2 + A(2)\bar{\rho}_1 \cdot \bar{\rho}_2 + A(3)\rho_2{}^2 + A(4)\bar{\rho}_1 \cdot \bar{\rho}_3 + A(5)\bar{\rho}_2 \cdot \bar{\rho}_3$$
$$+ A(6)\rho_3{}^2 + A(7)\bar{\rho}_1 \cdot \bar{\rho}_4 + A(8)\bar{\rho}_1 \cdot \bar{\rho}_4 + A(9)\bar{\rho}_3 \cdot \bar{\rho}_4 + A(10)\rho_4{}^2$$
$$+ A(11)\bar{\rho}_1 \cdot \bar{\rho}_3 + A(12)\bar{\rho}_2 \cdot \bar{\rho}_3 + A(13)\bar{\rho}_3 \cdot \bar{\rho}_5 + A(14)\bar{\rho}_4 \cdot \bar{\rho}_5 + A(15)\rho_5{}^2$$

$A(1) = B(k,6)$

$A(2) = B(k,13)$

$A(3) = B(k,15)$

$A(4) = B(k,4)$

$A(5) = B(k,11)$

$A(6) = B(k,1)$

$A(7) = B(k,5)$

$A(8) = B(k,12)$

$A(9) = B(k,2)$

$A(10) = B(k,3)$

$A(11) = B(k,4)$

$A(12) = B(k,14)$

$A(13) = B(k,7)$

$A(14) = B(k,8)$

$A(15) = B(k,10)$

Next the transformation which removes the cross terms in the exponent is

$$\bar{\rho}_1 = \bar{r}_1$$

$$\bar{\rho}_2 = E(2)\bar{r}_1 + \bar{r}_2$$

$$\bar{\rho}_3 = E(4)\bar{r}_1 + E(5)\bar{r}_2 + \bar{r}_3$$

$$\bar{\rho}_4 = E(7)\bar{r}_1 + E(8)\bar{r}_2 + E(9)\bar{r}_3 + \bar{r}_4$$

$$\bar{\rho}_5 = E(11)\bar{r}_1 + E(12)\bar{r}_2 + E(13)\bar{r}_3 + E(14)\bar{r}_4 + \bar{r}_5 \qquad \text{(B-6)}$$

under which the integral becomes

$$\langle(12345)|(1234;5)\rangle = |J|^3 \int \exp(-E(1)r_1^2 - E(3)r_2^2 - E(6)r_3^2 - E(10)r_4^2 - E(15)r_5^2)\, r_1 Y_1^{m*}(\Omega_1)\, [E(2) r_1 Y_1^m(\Omega_1) + r_2 Y_1^m(\Omega_2)]\, d\bar{r}_1\, d\bar{r}_2\, d\bar{r}_3\, d\bar{r}_4\, d\bar{r}_5 \qquad \text{(B-7)}$$

It remains a simple problem to show that this integral is reduced to

$$\langle(12345)_1|(1234;5)\rangle \pm \frac{24\pi^{13/2}\, E(2)}{E(1)\,[E(1)\, E(3)\, E(10)\, E(15)]^{3/2}} \qquad \text{(B-8)}$$

The only step which is unique for any particular configuration is the definition of the A's in terms of the B's as in eq. (B-5). This will be summarised in Table 7.

B.2 THE SECOND EXCITED STATE

The principles followed in the evaluation of the integrals for the second excited state are the

TABLE 7

TRANSFORMATION USED IN THE OVERLAP INTEGRALS INVOLVING THE GROUND STATE

A(1)	$(1s)^4(1p)$	$(1s)^3(1p)(2s)$	$(1s)^4(2p)$ $(1s)^4(3p)$
1	6	3	15
2	13	5	13
3	15	6	6
4	4	12	11
5	11	13	4
6	1	15	1
7	5	2	12
8	12	4	5
9	2	11	2
10	3	1	3
11	9	8	14
12	14	9	9
13	7	14	7
14	8	7	8
15	10	10	10

the same as for the ground state. For this state, however, there are three integrals per configuration. These are the direct, one-, and two-particle exchange terms. As an example, consider the $(1s)^3(1p)^2$ configuration.

The single-particle representation of the direct term is given in eq. (3-6). Introducing the relative coordinate by the transformation

$$\begin{aligned}
\bar{\xi}_1 &= \bar{r}_1 \\
\bar{\xi}_2 &= \bar{r}_2 \\
\bar{\xi}_3 &= +\tfrac{1}{3}\bar{r}_1 + \tfrac{1}{3}\bar{r}_2 + \tfrac{1}{3}\bar{r}_3 - \tfrac{1}{2}\bar{r}_4 - \tfrac{1}{2}\bar{r}_5 \\
\bar{\xi}_4 &= \bar{r}_4 \\
\bar{\xi}_5 &= \bar{r}_5
\end{aligned} \qquad \text{(B-9)}$$

reduces eq. (3-6) to

$$\langle (12345)_1 | (123;45) \rangle = |J|^3 \int e^{-\varphi_1}\, \bar{\xi}_2^{\,2}\, \bar{\xi}_4 \cdot \bar{\xi}_5 \; d\bar{\xi}_1\, d\bar{\xi}_2\, d\bar{\xi}_3\, d\bar{\xi}_4\, d\bar{\xi}_5 \qquad \text{(B-10)}$$

where

$$\varphi_1 = B(1,1)\xi_1^2 + B(1,2)\bar{\xi}_1\cdot\bar{\xi}_2 + B(1,3)\xi_2^2 + B(1,4)\bar{\xi}_1\cdot\bar{\xi}_3 + B(1,5)\bar{\xi}_2\cdot\bar{\xi}_3 + B(1,6)\xi_3^2 + B(1,7)\bar{\xi}_1\cdot\bar{\xi}_4 + B(1,8)\bar{\xi}_2\cdot\bar{\xi}_4$$

$$+ B(1,9)\bar{\xi}_2\cdot\bar{\xi}_4 + B(1,10)\xi_4^{\,2} + B(1,11)\bar{\xi}_1\cdot\bar{\xi}_5 + B(1,12)\bar{\xi}_2\cdot\bar{\xi}_5$$

$$+ B(1,13)\bar{\xi}_3\cdot\bar{\xi}_5 + B(1,14)\bar{\xi}_4\cdot\bar{\xi}_5 + B(1,15)\xi_5^{\,2}$$

$$B(1,1) = 2P - R$$

$$B(1,2) = 2P - R$$

$$B(1,3) = 2P - R$$

$$B(1,4) = -6P + 3R$$

$$B(1,5) = -6P + 3R$$

$$B(1,6) = 9P$$

$$B(1,7) = -3P + \frac{3}{2}R$$

$$B(1,8) = -3P + \frac{3}{2}R$$

$$B(1,9) = 9P + 3S$$

$$B(1,10) = Q + \frac{9}{4}P + \frac{3}{2}S$$

$$B(1,11) = -3P + \frac{3}{2}R$$

$$B(1,12) = -3P + \frac{3}{2}R$$

$$B(1,13) = 9P + 3S$$

$$B(1,14) = T + \frac{9}{2}P + 3S$$

$$B(1,15) = Q + \frac{9}{4}P + \frac{3}{2}S$$

$$P = \frac{\alpha}{3} + \frac{\beta}{15} + \frac{3\mu}{5}$$

$$R = -\frac{\alpha}{3} + \frac{\beta}{15} + \frac{\mu}{5}$$

$$Q = \frac{\bar{\alpha}}{4} + \frac{3\beta}{20} + \frac{3\mu}{5}$$

$$S = \frac{1}{5}(\mu - \beta)$$

$$T = -\frac{\bar{\alpha}}{2} + \frac{3\beta}{10} + \frac{\mu}{5}$$

$$J = \frac{\partial(\bar{\zeta}_1, \bar{\zeta}_2, \bar{\zeta}_3, \bar{\zeta}_4, \bar{\zeta}_5)}{\partial(\bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4, \bar{r}_5)} = \frac{1}{3}$$

The single-particle representation of the one-particle exchange integral is given in eq. (3-7). The transformation

$$\begin{aligned}
\bar{\xi}_1 &= \bar{r}_1 \\
\bar{\xi}_2 &= \bar{r}_3 \\
\bar{\xi}_3 &= +\frac{1}{3}\bar{r}_1 + \frac{1}{3}\bar{r}_2 - \frac{1}{2}\bar{r}_3 + \frac{1}{3}\bar{r}_4 - \frac{1}{2}\bar{r}_5 \\
\bar{\xi}_4 &= \bar{r}_4 \\
\bar{\xi}_5 &= \bar{r}_5 \qquad \text{(B-11)}
\end{aligned}$$

introduces the one-particle exchange relative coordinate, under which (3-7) assumes the form (B-10) where

$$\begin{aligned}
\varphi_1 = {} & B(2,1)\xi_1{}^2 + B(2,2)\bar{\xi}_1 \cdot \bar{\xi}_2 + B(2,3)\xi_2{}^2 + B(2,4)\bar{\xi}_1 \cdot \bar{\xi}_3 \\
& + B(2,5)\bar{\xi}_2 \cdot \bar{\xi}_3 + B(2,6)\xi_3{}^2 + B(2.7)\bar{\xi}_1 \cdot \bar{\xi}_4 + B(2,8)\bar{\xi}_2 \cdot \bar{\xi}_4 \\
& + B(2,9)\bar{\xi}_2 \cdot \bar{\xi}_4 + B(2,10)\xi_4{}^2 + B(2,11)\bar{\xi}_1 \cdot \bar{\xi}_5 + B(2,12)\bar{\xi}_2 \cdot \bar{\xi}_5 \\
& + B(2,13)\bar{\xi}_3 \cdot \bar{\xi}_5 + B(2,14)\bar{\xi}_4 \cdot \bar{\xi}_5 + B(2,15)\xi_5{}^2
\end{aligned}$$

$$B(2,1) = 2P - R$$

$$B(2,2) = -3P + \frac{3}{2}R$$

$$B(2,3) = Q + \frac{9}{4}P + \frac{3}{2}S$$

$$B(2,4) = -6P + 3R$$

$$B(2,5) = 9P + 3S$$

$$B(2,6) = 9P$$

$$B(2,7) = 2P - R$$

$$B(2,8) = -3P + \frac{3}{2}R$$

$$B(2,9) = -6P + 3R$$

$$B(2,10) = 2P - R$$

$$B(2,11) = 9P + 3S$$

$$B(2,12) = T + \frac{9}{2}P + 3S$$

$$B(2,13) = 9P + 3S$$

$$B(2,14) = -3P + \frac{3}{2}R$$

$$B(2,15) = Q + \frac{9}{4}P + \frac{3}{2}S$$

Finally, the two-particle exchange integral (3-8) is transformed into the form (B-10) by

$$\bar{\xi}_1 = \bar{r}_1$$
$$\bar{\xi}_2 = -\frac{1}{2}\bar{r}_1 + \frac{1}{3}\bar{r}_2 - \frac{1}{2}\bar{r}_3 + \frac{1}{3}\bar{r}_4 + \frac{1}{3}\bar{r}_5$$

(B-12) con't

$$\bar{\xi}_3 = \bar{r}_3$$

$$\bar{\xi}_4 = \bar{r}_4$$

$$\bar{\xi}_5 = \bar{r}_5$$

where

$$\varphi_1 = B(3,1)\xi_1^2 + B(3,2)\bar{\xi}_1\cdot\bar{\xi}_2 + B(3,3)\xi_2^2 + B(3,4)\bar{\xi}_1\cdot\bar{\xi}_3$$

$$+ B(3,5)\bar{\xi}_2\cdot\bar{\xi}_3 + B(3,6)\xi_3^2 + B(3,7)\overline{\xi_1\cdot\xi_4} + B(3,8)\bar{\xi}_2\cdot\bar{\xi}_4$$

$$+ B(3,9)\bar{\xi}_2\cdot\bar{\xi}_4 + B(3,10)\xi_4^2 + B(3,11)\bar{\xi}_1\cdot\bar{\xi}_5 + B(3,12)\bar{\xi}_2\cdot\bar{\xi}_5$$

$$+ B(3,13)\bar{\xi}_3\cdot\bar{\xi}_3 + B(3,14)\bar{\xi}_4\cdot\bar{\xi}_5 + B(3,15)\xi_5^2$$

$$B(3,1) = Q + \frac{9}{4}P + \frac{3}{2}S$$

$$B(3,2) = T + \frac{9}{2}P + 3S$$

$$B(3,3) = Q + \frac{9}{4}P + \frac{3}{2}S$$

$$B(3,4) = 9P + 3S$$

$$B(3,5) = 9P + 3S$$

$$B(3,6) = 9P$$

$$B(3,7) = -3P + \frac{3}{2}R$$

$$B(3,8) = -3P + \frac{3}{2}R$$

$$B(3,9) = -6P + 3R$$

$$B(3,10) = 2P - R$$

$$B(3,11) = -3P + \frac{3}{2}R$$

$$B(3,12) = -3P + \frac{3}{2}R$$

$$B(3,13) = -3P + \frac{3}{2}R$$

$$B(3,14) = 2P - R$$

$$B(3,15) = 2P - R$$

The remaining steps are analoqous to those of the ground state calculation. They are summarized in Table 6.

TABLE 8

TRANSFORMATION USED IN THE OVERLAP INTEGRALS INVOLVING THE SECOND EXCITED STATE.

A(1)	$(1s)^3(1p)^2$ $(1s)^3(1p)(2p)$ $(1s)^3(2p)^2$	$(1s)^2(1p)^2(2s)$
1	6	6
2	9	4
3	10	1
4	13	9
5	14	7
6	15	10
7	4	13
8	7	11
9	11	14
10	1	15
11	5	5
12	8	2
13	12	8
14	2	12
15	3	3

APPENDIX C

THE REDUCTION OF THE EXPONENT (2,14)

Given the quadratic form

$$\varphi = A(1)r_1{}^2 + A(2)\bar{r}_1\cdot\bar{r}_2 + A(3)r_2{}^2 + A(4)\bar{r}_1\cdot\bar{r}_3 + A(5)\bar{r}_2\cdot\bar{r}_3$$

$$+ A(6)r_3{}^2 + A(7)\bar{r}_1\cdot\bar{r}_4 + A(8)\bar{r}_2\cdot\bar{r}_4 + A(9)\bar{r}_3\cdot\bar{r}_4 + A(10)r_4{}^2$$

$$+ A(11)\bar{r}_1\cdot\bar{r}_5 + A(12)\bar{r}_2\cdot\bar{r}_3 + A(13)\bar{r}_3\cdot\bar{r}_5 + A(14)\bar{r}_4\cdot\bar{r}_5$$

$$+ A(15)r_5{}^2 \quad ; \tag{C-1}$$

the problem was to eliminate all the cross terms. This has been accomplished by a series of five transformations, each of which eliminates one set of cross terms. The first transformation eliminates all cross terms involving $\bar{r}_5$

$$\bar{\xi}_1 = \bar{\mathbf{r}}_1$$

$$\bar{\xi}_2 = \bar{r}_2$$

$$\bar{\xi}_3 = \bar{r}_3$$

$$\bar{\xi}_4 = \bar{r}_4$$

$$\bar{\xi}_5 = \bar{r}_5 + \frac{A(1)}{2A(15)}\,\bar{r}_1 + \frac{A(12)}{2A(15)}\,\bar{r}_2 + \frac{A(3)}{2A(15)}\,\bar{r}_3$$

$$+ \frac{A(14)}{2A(15)}\,\bar{r}_4 \tag{C-2}$$

This transforms φ into

$$\varphi = B(1)\xi_1^2 + B(2)\bar{\xi}_1 \cdot \bar{\xi}_2 + B(3)\xi_2^2 + B(4)\bar{\xi}_1 \cdot \bar{\xi}_3 + B(5)\bar{\xi}_2 \cdot \bar{\xi}_3$$

$$+ B(6)\xi_3^2 + B(7)\bar{\xi}_1 \cdot \bar{\xi}_4 + B(8)\bar{\xi}_2 \cdot \bar{\xi}_4 + B(9)\bar{\xi}_3 \cdot \bar{\xi}_4 + B(10)\xi_4^2$$

$$+ A(15)\xi_5^2 \qquad (C-3)$$

where

$$B(1) == A(1) - \frac{(A(11))^2}{4A(15)}$$

$$B(2) = A(2) - \frac{A(11)\ A(12)}{2A(15)}$$

$$B(3) = A(3) - \frac{(A(12))^2}{4A(15)}$$

$$B(4) = A(4) - \frac{A(11)\ A(13)}{2A(15)}$$

$$B(5) = A(5) - \frac{A(12)\ A(13)}{2A(15)}$$

$$B(6) = A(6) - \frac{(A(13))^2}{4A(15)}$$

$$B(7) = A(7) - \frac{A(11)\ A(12)}{2A(15)}$$

$$B(8) = A(8) - \frac{A(12)\ A(14)}{2A(15)}$$

$$B(9) = A(9) - \frac{A(13)\ A(14)}{2A(15)}$$

$$B(10) = A(10) - \frac{(A(14))^2}{4A(15)}$$

The next transformation is chosen to eliminate all cross terms involving $\bar{\xi}_4$

$$
\begin{aligned}
\bar{\zeta}_1 &= \bar{\xi}_1 \\
\bar{\zeta}_2 &= \bar{\xi}_2 \\
\bar{\zeta}_3 &= \bar{\xi}_3 \\
\bar{\zeta}_4 &= \bar{\xi}_4 + \frac{B(7)}{2B(10)}\bar{\xi}_1 + \frac{B(8)}{2B(10)}\bar{\xi}_2 + \frac{B(9)}{2B(10)}\bar{\xi}_3 \\
\bar{\zeta}_5 &= \bar{\xi}_5
\end{aligned}
\tag{C-4}
$$

Upon application of this transformation, φ is reduced to

$$
\varphi = C(1)\zeta_1^2 + C(2)\bar{\zeta}_1 \cdot \bar{\zeta}_2 + C(3)\zeta_2^2 + C(4)\bar{\zeta}_1 \cdot \bar{\zeta}_3 + C(5)\bar{\zeta}_2 \cdot \bar{\zeta}_3 + C(6)\bar{\zeta}_3^2 + B(10)\zeta_4^2 + A(15)\zeta_5^2
$$

where

$$
\begin{aligned}
C(1) &= B(1) - \frac{(B(7))^2}{4B(10)} \\
C(2) &= B(2) - \frac{B(7)\ B(8)}{2B(10)} \\
C(3) &= B(3) - \frac{(B(8))^2}{4B(10)} \\
C(4) &= B(4) - \frac{B(7)\ B(9)}{2B(10)} \\
C(5) &= B(5) - \frac{B(8)\ B(9)}{2B(10)} \\
C(6) &= B(6) - \frac{(B(9))^2}{4B(10)}
\end{aligned}
$$

The following transformation is used to eliminate cross terms involving $\bar{\xi}_3$

$$\bar{\eta}_1 = \bar{\xi}_1$$

$$\bar{\eta}_2 = \bar{\xi}_2$$

$$\bar{\eta}_3 = \bar{\xi}_3 + \frac{C(4)}{2C(6)}\bar{\xi}_1 + \frac{C(5)}{2C(6)}\bar{\xi}_2$$

$$\bar{\eta}_4 = \bar{\xi}_4$$

$$\bar{\eta}_5 = \bar{\xi}_5 \qquad \text{(C-6)}$$

Applying this to φ gives

$$\varphi = D(1)\eta_1{}^2 + D(2)\bar{\eta}_1 \cdot \bar{\eta}_2 + D(3)\eta_2{}^2 + C(6)\eta_3{}^2 + B(10)\eta_4{}^2 + A(15)\eta_5{}^2 \qquad \text{(C-7)}$$

where

$$D(1) = C(1) - \frac{(C(4))^2}{4C(6)}$$

$$D(2) = C(2) - \frac{C(4)\ C(5)}{2C(6)}$$

$$D(3) = C(3) - \frac{(C(5))^2}{4C(6)}$$

The last cross term can be eliminated by

$$\bar{\rho}_1 = \bar{\eta}_1$$

$$\bar{\rho}_2 = \bar{\eta}_2 + \frac{D(2)}{2D(3)}\bar{\eta}_1$$

$$\bar{\rho}_3 = \bar{\eta}_3$$

$$\bar{\rho}_4 = \bar{\eta}_4$$

$$\bar{\rho}_5 = \bar{\eta}_5 \qquad \text{(C-8)}$$

Thus, the form of φ with no cross terms is

$$\varphi = E(1)\rho_1^2 + E(3)\rho_2^2 + E(6)\rho_3^2 + E(10)\rho_4^2 + E(15)\rho_5^2 \tag{C-9}$$

Solving for the $\bar{r}$'s in terms of the $\bar{\rho}$'s, the complete transformation is

$$\begin{aligned}
\bar{r}_1 &= \bar{\rho}_1 \\
\bar{r}_2 &= E(2)\bar{\rho}_1 + \bar{\rho}_2 \\
\bar{r}_3 &= E(4)\bar{\rho}_1 + E(5)\bar{\rho}_2 + \bar{\rho}_3 \\
\bar{r}_4 &= E(7)\bar{\rho}_1 + E(8)\bar{\rho}_2 + E(9)\bar{\rho}_3 + \bar{\rho}_4 \\
\bar{r}_5 &= E(11)\bar{\rho}_1 + E(12)\bar{\rho}_2 + E(13)\bar{\rho}_3 + E(14)\bar{\rho}_4 + \bar{\rho}_5
\end{aligned} \tag{C-10}$$

where

$$E(1) = D(1) - \frac{(D(2))^2}{4D(3)}$$

$$E(2) = -\frac{D(2)}{2D(3)}$$

$$E(3) = D(3)$$

$$E(4) = -\frac{1}{2C(6)}[C(4) - E(2)C(5)]$$

$$E(5) = -\frac{C(5)}{2C(6)}$$

$$E(6) = C(6)$$

$$E(7) = -\frac{[B(7) + B(8)\ E(2) + B(9) E(4)]}{2B(10)}$$

$$E(8) = -\frac{B(8) + B(9)\ E(5)]}{2B(10)}$$

$$E(9) = -\frac{B(9)}{2B(10)}$$

$$E(10) = B(10)$$

$$E(11) = -\frac{[A(11) + A(12)\ E(2) + A(13)\ E(4) + A(14)\ E(7)]}{2A(15)}$$

$$E(12) = -\frac{[A(17) + A(13)\ E(5) + A(19)\ E(9)]}{2\ A(15)}$$

$$E(13) = -\frac{[A(13) + A(14)\ E(9)]}{2\ A(15)}$$

$$E(14) = -\frac{A(14)}{2A(15)}$$

$$E(15) = A(15)$$

It should be noted that

$$\frac{\partial(\bar{\rho}_1, \bar{\rho}_2, \bar{\rho}_3, \bar{\rho}_4, \bar{\rho}_5)}{\partial(\bar{r}_1, \bar{r}_2, \bar{r}_3, \bar{r}_4, \bar{r}_5)} = 1 \tag{C-11}$$

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