

CONFIGURATION MIXING IN THE CLUSTER MODEL  
WAVE FUNCTIONS OF THE  $\text{He}^5$  NUCLEUS

by

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TO MY PARENTS

## ABSTRACT

The admixture of harmonic oscillator shell model states in the cluster model wave functions has been calculated for the ground state ( $3/2^-$ ) and the second excited state ( $3/2^+$ ) of  $\text{He}^5$ . The sensitivity of the configuration mixing in the ground state to variations of the cluster model width parameters has also been calculated and discussed. Some other features of the cluster model wave functions have also been discussed briefly.

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The admixture of harmonic oscillator shell model states in the cluster model wave functions has been calculated for the ground state ( $3/2^-$ ) and the second excited state ( $3/2^+$ ) of  $\text{He}^5$ . The sensitivity of the configuration mixing in the ground state to variations of the cluster model width parameters has also been calculated and discussed. Some other features of the cluster model wave functions have also been discussed briefly.

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TABLE OF CONTENTS

ABSTRACT-----iv

ACKNOWLEDGEMENTS-----v

LIST OF ILLUSTRATIONS-----vii

LIST OF TABLES-----viii

Chapter I. Introduction----- 1

Chapter II. Expansion of the Cluster Model Wave Function of  
the Ground State----- 9

Chapter III. Expansion of the Cluster Model Wave Function of  
the Second Excited State-----18

Chapter IV. Conclusion and Discussion-----28

Appendix I. Evaluation of Integrals of the Type  
 $\int (\vec{r}Br) e^{-\vec{r}Ar} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$ -----37

Appendix II. Evaluation of Integrals of the Type  
 $\int (\vec{r}Br) (\vec{r}Cr) e^{-\vec{r}Ar} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$ -----41

Appendix III. Normalization Constants-----44

Appendix IV. The Equivalence of the Cluster Model and the  
HCSM Wave Functions-----47

LIST OF ILLUSTRATIONS

Fig. 1. Harmonic Oscillator Potential Well for the HOSM----- 3

Fig. 2. The Intensities of the Different Configurations  
Found in the Ground State Cluster Model Wave  
Function with Constant  $\alpha_1$ , as Functions of  
 $\beta'$  -----50

Fig. 3. The Intensities of the Different Configurations  
Found in the Ground State Cluster Model Wave  
Function with Constant  $\beta'$ , as Functions of  
 $\alpha_1$  -----51

Fig. 4. The Intensities of the Different Configurations  
Found in the Ground State Cluster Model Wave  
Function with Constant  $\alpha_1 = \mu_1$ , as Functions  
of  $\beta'$  -----52

LIST OF TABLES

- Table 1. The Width Parameters for the Cluster Model and  
HOSM Wave Functions-----11
- Table 2. The Intensities of the Different Configurational  
States Found in the Ground State Cluster  
Model Wave Function with Width Parameters:  
 $\alpha_1 = 4.33 \times 10^{25} \text{cm}^{-2}$ ,  $\beta' = \begin{Bmatrix} 2.25 \\ 3.25 \end{Bmatrix} \times 10^{25} \text{cm}^{-2}$  and  
 $\mu_1 = 3.65252 \times 10^{25} \text{cm}^{-2}$ -----31
- Table 3. The Intensities of the Different Configurational  
States Found in the Second Excited State  
Cluster Model Wave Function with Width Para-  
meters:  $\alpha = 2.81 \times 10^{25} \text{cm}^{-2}$ ,  $\bar{\alpha} = 4.78 \times 10^{25} \text{cm}^{-2}$ ,  
 $\beta = 0.422 \times 10^{25} \text{cm}^{-2}$  and  $\mu_1 = 3.65252 \times 10^{25} \text{cm}^{-2}$ -----32

## CHAPTER I

### Introduction

In the past decade the cluster model has achieved some success in predicting the low-lying energy levels of certain light nuclei (1). This thesis will be concerned especially with the cluster model representation of the  $\text{He}^5$  nucleus. Pearlstein et al (2) have demonstrated that good results for the energies of the first three levels in  $\text{He}^5$  are obtained when the cluster model is used. Also, Tran Duc and Smith (3) have calculated the radiative transition probability from the  $3/2^+$  (second excited) state to the  $3/2^-$  (ground) state in  $\text{He}^5$ , and obtain a result which is in quite close agreement with the experimental value. There are therefore some indications that the cluster model wave functions provide a good description of the  $\text{He}^5$  nucleus.

In the cluster model, different spatial correlations between nucleons may be favoured in different nuclear states. On the other hand, the harmonic oscillator shell model (HOSM) treats the nucleons in a nucleus as independent particles moving in a common harmonic oscillator potential well. The HOSM thus includes no spatial correlations between nucleons in the nucleus at all.

In the cluster model, the ground state of  $\text{He}^5$  is assumed to consist of an alpha particle and a neutron, the state of whose relative motion is a  $1p$  state (2). The second excited state has a different cluster structure, and can be described as consisting of a triton and a deuteron; the state

of the relative motion of the deuteron and the triton is a 2s state (2). Here it should be noted that the deuteron cluster, the triton cluster and the alpha particle cluster are energetically in their ground states (1).

The cluster model spatial wave function of the ground state is (2)

$$\phi(3/2^-) = \exp(-\frac{1}{2}\alpha_1 \sum_{i=1}^4 \vec{r}_i'^2) \vec{R}_1 Y_1^m(\Omega_1) \exp(-\frac{2}{5}\beta' \vec{R}_1^2) \exp(-\frac{5}{2}\mu_1 \vec{R}_{cm}^2) \quad (I-1)$$

where

$$\vec{r}_i' = \vec{r}_i - \frac{1}{4} \sum_{j=1}^4 \vec{r}_j, \quad \vec{R}_1 = \frac{1}{4} \sum_{j=1}^4 \vec{r}_j - \vec{r}_5, \quad \vec{R}_{cm} = \frac{1}{5} \sum_{j=1}^5 \vec{r}_j. \quad (2)$$

The spatial wave function of the second excited state is

$$\phi(3/2^+) = \exp(-\frac{1}{2}\alpha \sum_{i=1}^3 \vec{r}_i''^2 - \frac{1}{2}\bar{\alpha} \sum_{j=4}^5 \vec{r}_j''^2) \vec{R}^2 \exp(-\frac{3}{5}\beta \vec{R}^2) \exp(-\frac{5}{2}\mu_1 \vec{R}_{cm}^2) \quad (I-2)$$

where

$$\vec{r}_i'' = \vec{r}_i - \frac{1}{3} \sum_{k=1}^3 \vec{r}_k, \quad \vec{r}_j'' = \vec{r}_j - \frac{1}{2} \sum_{k=4}^5 \vec{r}_k, \quad \vec{R} = \frac{1}{3} \sum_{k=1}^3 \vec{r}_k - \frac{1}{2} \sum_{k=4}^5 \vec{r}_k.$$

Here the width parameters  $\alpha_1, \beta'$  for the ground state and  $\alpha, \bar{\alpha}, \beta$  for the second excited state were determined by a variational calculation of the energies of these states (2).

The width parameter  $\mu_1$ , associated with the (fictitious) center of mass motion is chosen to be the same as that in the shell model calculation (4).

The HOSM spatial wave function is a direct product of the individual spatial wave function of the individual nucleons, each of which moves in the common harmonic oscillator potential. Thus, the HOSM spatial wave function is

$$\phi(L^\pi) = \phi(1_1^{\pi_1}) \phi(1_2^{\pi_2}) \dots \phi(1_A^{\pi_A})$$

where

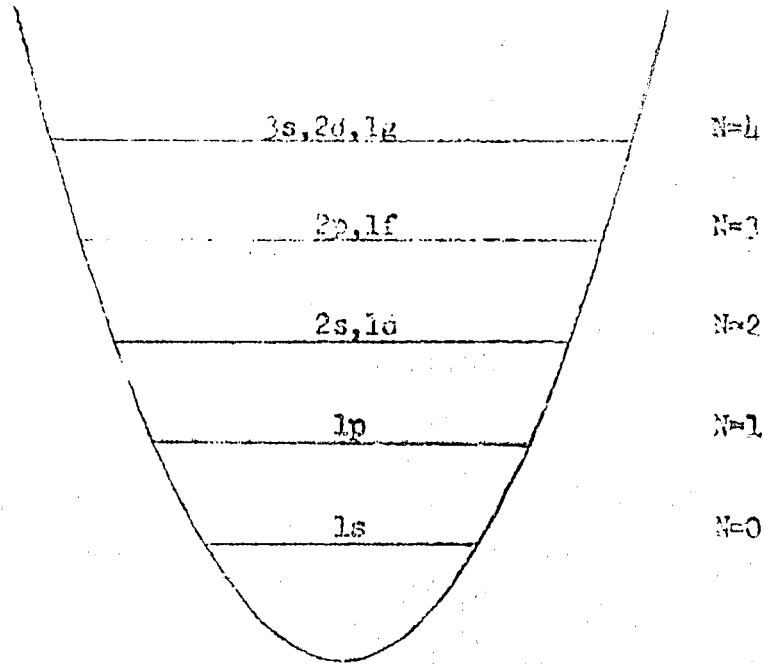


Fig. 1 Harmonic Oscillator Potential Well for the  
HOSM.

$$\phi(l_i \pi_i) = \exp(-\frac{1}{2}\mu_i r_i^2) r_i^{l_i} L_{\frac{N-l_i}{2}}^{l_i+\frac{1}{2}}(\mu_i r_i^2) Y_{l_i}^{m_i}(\Omega_i) \quad (I-3)$$

Note that, since all the nucleons are moving in the same oscillator potential, the width parameter  $\mu_i$  is the same for all the individual spatial wave functions.

For the sake of convenience, the following notation will be used throughout this work. The cluster model spatial wave functions for the ground state eq.(I-1) and the second excited state eq.(I-2) are represented in the following way respectively:

$$\phi(3/2^-) = (1234; 5), \quad \phi(3/2^+) = (123; 45),$$

and the HOSM spatial wave functions are denoted by (12345).

The first two and the fifth positions represent the neutrons, while the third and fourth positions represent the protons.

The spin wave functions of the ground state of  $He^5$  in both models are identical; the total spin of the ground state is  $S = \frac{1}{2}$ , since it is formed by the coupling of the spins of two neutrons and two protons in the 1s spatial state (or in the cluster model language, an alpha particle cluster), which is zero, and the spin of the last single neutron. The spin wave function can therefore be chosen to be (5)

$$\chi_- = \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5$$

The cluster model spin wave function for the second excited state is formed by coupling the spin of the triton and the spin of the deuteron. As was shown in Tran Duc's work (5), there are four different possible sets of spin wave functions. One of them has to be ruled out because it violates the

Pauli principle. Two others give a vanishing electric dipole matrix element, and so are arbitrarily disregarded. Thus the only spin wave function used here is (5)

$$\chi_+ = \frac{1}{\sqrt{6}} [ (\alpha_1 \beta_3 + \beta_1 \alpha_3) \alpha_2 - 2 \alpha_1 \beta_2 \alpha_3 ] \alpha_4 \alpha_5.$$

The same set of four possible spin states exists in the HOSM wave function for the second excited state as well. For the same reasons as were given above for the cluster model spin wave function, the same spin wave function is adopted for the HOSM.

In using the HOSM, it is correct to consider the nucleons moving in pure single-particle orbits only if there is no residual interaction in addition to the effective harmonic oscillator potential. In the absence of such a residual interaction, all states of  $k$  particles (having the same  $n, l, j$ ) in the same configuration will be degenerate. But in the actual nucleus, such interactions do exist. If a residual internucleon potential  $v_{ij}$  is introduced which is strong enough to remove the degeneracies, the energies of the state will change, and at the same time the wave functions will also be changed by the interaction. Such a mixed state can be represented as a superposition of the wave functions of several pure states (with same  $n, l, j$ ) whose energies are close to one another.

Since the eigenfunctions of different states in the HOSM are mutually orthogonal and form a complete set, then any wave function can be expanded in terms of these HOSM wave

functions. For instance, "individual particle model"\* wave functions, alpha-particle model wave functions (6), and cluster model wave functions (7) can be expanded in a sum of HOSM wave functions of all possible configurations.

Since the energy levels, nuclear magnetic moments (8), nuclear quadrupole moments (9), and so on, are quite sensitive to the configuration mixing of the HOSM wave functions, thus the configuration mixing in the "more realistic wave functions" may be helpful in obtaining better theoretical results. In the present work, the expansion of the cluster model wave functions as a linear combination of HOSM wave functions gives the equivalence between the cluster model wave functions and the shell model wave functions, in the sense in which configurations are mixed in calculations using the "individual particle model".

In order to expand the cluster model wave functions as a linear combination of the HOSM wave functions, the wave functions for both models must be antisymmetrized. The method of antisymmetrization used here differs from that of Kanellopoulos and Wildermuth (10) in that the proton and neutron functions are antisymmetrized separately (3,5). This method has two advantages; first, isospin need not be included in the wave functions, and second, the calculation of the expansion coefficients is simplified.

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\* Here the "individual particle model" means that in addition to the common harmonic oscillator potential well, some kind of residual internucleon interactions are included.

The antisymmetrization operator  $\mathcal{A}$  is (11)

$$\mathcal{A} = \mathcal{A}_n \mathcal{A}_p,$$

where

$$\mathcal{A}_n = \frac{1}{3!} \sum_{n=1,2,5} (-1)^{\pi} P_n, \quad \mathcal{A}_p = \frac{1}{2} \sum_{p=3,4} (-1)^{\pi} P_p,$$

$P$  is a permutation operator and  $(-1)^{\pi}$  is the parity of the permutation.

The antisymmetrized cluster model wave functions are

$$\underline{\Phi}(3/2-) = \mathcal{A} \phi(3/2-) = N_- \mathcal{A} \{ (1234; 5) \chi_- \},$$

$$\underline{\Phi}(3/2+) = \mathcal{A} \phi(3/2+) = N_+ \mathcal{A} \{ (123; 45) \chi_+ \}.$$

The normalization constants for both model wave functions are determined from equations of the form

$$\langle \underline{\Phi} | \underline{\Phi} \rangle = \langle \phi | \phi \rangle = 1. \quad (\text{I-4})$$

The simplification occurs because  $\mathcal{A}$  is idempotent (i.e.,  $\mathcal{A}^2 = \mathcal{A}$ ).

If the cluster model wave function  $|\phi_{CM}\rangle$  are expanded in a linear combination of the HOSM wave functions of different configurations  $|\phi_{SMi}\rangle$  (where  $J$  and  $\pi$  are the same as in  $|\phi_{CM}\rangle$ ; also  $i$  labels the different configurations), then

$$|\phi_{CM}\rangle = a_1 |\phi_{SM1}\rangle + a_2 |\phi_{SM2}\rangle + \dots + a_i |\phi_{SMi}\rangle + \dots \quad (\text{I-5})$$

Applying the antisymmetrization operator  $\mathcal{A}$  to eq.(I-5), there results

$$|\underline{\Phi}_{CM}\rangle = a_1 |\underline{\Phi}_{SM1}\rangle + a_2 |\underline{\Phi}_{SM2}\rangle + \dots + a_i |\underline{\Phi}_{SMi}\rangle + \dots \quad (\text{I-6})$$

Since the HOSM wave functions satisfy the orthonormality condition

$$\langle \phi_{SMj} | \mathcal{A} \phi_{SMi} \rangle = \delta_{ji}, \quad (\text{I-7})$$

then the expansion coefficient  $a_i$  can be obtained by taking the scalar product of  $|\phi_{SMi}\rangle$  with  $|\Phi_{CM}\rangle$ :

$$\langle \phi_{SMi} | \mathcal{A} \phi_{CM} \rangle = a_i. \quad (\text{I-8})$$

Since the cluster model wave functions are normalized as shown in eq.(I-4), then from eqs.(I-5),(I-6) and (I-7) there results

$$\langle \phi_{CM} | \mathcal{A} \phi_{CM} \rangle = \sum_i |a_i|^2 = 1. \quad (\text{I-9})$$

This is a condition on the expansion coefficients which must be satisfied; it provides a check which indicates when a sufficient number of configurations has been included. The square of the amplitude  $|a_i|^2$  is physically more interesting than the expansion coefficient  $a_i$ ; it gives directly the weight of the HOSM state  $i$  in the cluster model wave function.

In Chapter II and III the HOSM expansions of the cluster model wave functions for the ground state and the second excited state of  $\text{He}^5$  will be studied.

In Chapter IV the width parameters in the ground state cluster model wave function will be varied and the corresponding expansion amplitudes calculated. By comparing these results with those given in Chapter II, the sensitivity of the expansion coefficients to variations of the width parameters can be determined.

CHAPTER II

Expansion of the Cluster Model Wave Function  
of the Ground State

1. The HOSM Scheme

The HOSM represents the ground state of  $\text{He}^5$  as consisting of two neutrons and two protons in the 1s level and one neutron in the 1p level [denoted in the usual spectroscopic notation as  $(1s)^4(1p)^1$ ]. The 1p neutron has one quantum of energy  $\hbar\omega$  relative to the 1s level.

Using the L-S coupling scheme, the four 1s nucleons couple to give zero spin and orbital angular momentum, and the 1p nucleon has  $s=\frac{1}{2}$ ,  $l=1$ , which forms the total angular momentum and parity  $J=3/2^-$ . However, as stated in Ch.I, the ground state of  $\text{He}^5$  consists not only of the  $(1s)^4(1p)^1$  configuration, but also has some contributions from the configurations having two quanta of excitation or even four quanta of excitation above the  $(1s)^4(1p)^1$  state.

The configurations having two and four quanta of excitation above the  $(1s)^4(1p)^1$  state, and which have the same total angular momentum and parity, are

Two quanta of excitation:

$$(1s)^{-1}(2s)^1, \quad (1s)^{-1}(1d)^1, \quad (1s)^{-2}(1p)^2, \quad (1p)^{-1}(2p)^1;$$

Four quanta of excitation:

$$(1s)^{-2}(2s)^2, \quad (1s)^{-2}(2s)^1(1d)^1, \quad (1s)^{-1}(3s)^1, \quad (1p)^{-1}(3p)^1,$$

$$(1s)^{-1}(1p)^{-1}(2s)^1(2p)^1, \quad (1s)^{-1}(2d)^1.$$

## 2. The General Formula for the Expansion Coefficients

The unantisymmetrized HOSM wave function for the ground state of  $\text{He}^5$  is

$$\phi_{\text{SMI}} = N_{\text{SMI}} (12345)_i \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \quad (\text{II-1})$$

The antisymmetrized HOSM wave function is obtained by applying the antisymmetrization operator  $\mathcal{A}$  to eq.(II-1):

$$\begin{aligned} \mathcal{A} \phi_{\text{SMI}} = \frac{N_{\text{SMI}}}{12} (\alpha_3 \beta_4 - \beta_3 \alpha_4) \{ & (\alpha_1 \beta_2 - \beta_1 \alpha_2) \alpha_5 (12345)_i \\ & - \alpha_1 (\beta_2 \alpha_5 - \alpha_2 \beta_5) (52341)_i + \alpha_2 (\beta_1 \alpha_5 - \alpha_1 \beta_5) (15342)_i \} . \end{aligned} \quad (\text{II-2})$$

Here again the subscript  $i$  on the wave function, the normalization constant and the spatial wave function designates the various configurations.

The unantisymmetrized cluster model wave function for the ground state of  $\text{He}^5$  is

$$\phi_{\text{CM}} = N_{\text{CM}} (1234;5) \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5, \quad (\text{II-3})$$

and the antisymmetrized cluster model wave function is

$$\begin{aligned} \mathcal{A} \phi_{\text{CM}} = \frac{N_{\text{CM}}}{12} (\alpha_3 \beta_4 - \beta_3 \alpha_4) \{ & (\alpha_1 \beta_2 - \beta_1 \alpha_2) \alpha_5 (1234;5) \\ & - \alpha_1 (\beta_2 \alpha_5 - \alpha_2 \beta_5) (5234;1) + \alpha_2 (\beta_1 \alpha_5 - \alpha_1 \beta_5) (1534;2) \} . \end{aligned} \quad (\text{II-4})$$

The normalization constants for both model wave functions are determined by using eq.(I-1). The numerical results of these

calculations are given in App. III.

From eq.(I-8) the expansion coefficients  $a_i$  can be obtained, as can be seen from the following equation,

$$a_i = \langle \phi_{SMI} | \mathcal{A} \phi_{CM} \rangle$$

$$= \frac{N_{SMI} N_{CM}}{12} \{ \langle (12345)_i | (1234;5) - (5234;1) \rangle \} \quad (II-5)$$

which is formed by taking the scalar product of eq.(II-1) with eq.(II-4). Equation (II-5) is a general equation which will be used throughout in the calculation of the expansion coefficients  $a_i$  for the ground state of  $He^5$ .

Before carrying out the calculation, the width parameters for the cluster model (2) and HOSM (4) wave functions will be given. These parameters are given in the following table.

Parameter	Value ( $10^{25} \text{cm}^{-2}$ )	Reference
$\mu_1$	3.65252	(4)
$\alpha_1$	4.33	(2)
$\beta'$	2.25 3.25	(2)
$\alpha$	2.81	(2)
$\bar{\alpha}$	4.78	(2)
$\beta$	0.422	(2)

Table 1. The width parameters for the cluster model and HOSM wave functions.

The two values for  $\beta'$  arise from two possible choices for the range and depth of the spin-orbit potential used in Ref. (2).

calculations are given in App. III.

From eq.(I-8) the expansion coefficients  $a_i$  can be obtained, as can be seen from the following equation,

$$a_i = \langle \phi_{SMI} | A \phi_{CM} \rangle$$

$$= \frac{N_{SMI} N_{CM}}{12} \{ \langle (12345)_i | (1234;5) - (5234;1) \rangle \} \quad (II-5)$$

which is formed by taking the scalar product of eq.(II-1) with eq.(II-4). Equation (II-5) is a general equation which will be used throughout in the calculation of the expansion coefficients  $a_i$  for the ground state of  $He^5$ .

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$\alpha$	2.81	(2)
$\bar{\alpha}$	4.78	(2)
$\beta$	0.422	(2)

Table 1. The width parameters for the cluster model and HOSM wave functions.

The two values for  $\beta'$  arise from two possible choices for the range and depth of the spin-orbit potential used in Ref. (2).

3. Numerical Calculation of Expansion Coefficients

(i). The HOSM spatial wave function for the configuration  $(1s)^4(1p)^1$  is

$$(12345)_1 = \exp\left(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2\right) \vec{r}_5 Y_1^1(\Omega_5).$$

Thus,

$$\langle (12345)_1 | (1234;5) \rangle$$

$$= \int \exp\left[-A(r_1^2+r_2^2+r_3^2+r_4^2) - Br_5^2 - C(\vec{r}_1 \cdot \vec{r}_2 + \vec{r}_1 \cdot \vec{r}_3 + \vec{r}_1 \cdot \vec{r}_4 + \vec{r}_2 \cdot \vec{r}_3 + \vec{r}_2 \cdot \vec{r}_4 + \vec{r}_3 \cdot \vec{r}_4) - D(\vec{r}_1 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_5 + \vec{r}_3 \cdot \vec{r}_5 + \vec{r}_4 \cdot \vec{r}_5)\right] \vec{r}_5 \cdot \left[\frac{1}{4}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_5\right] Y_1^{1*}(\Omega_5) Y_1^1(\Omega_{R_5}) \times d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

and

$$\langle (12345)_1 | (5234;1) \rangle$$

$$= \int \exp\left[-A(r_2^2+r_3^2+r_4^2+r_5^2) - Br_1^2 - C(\vec{r}_2 \cdot \vec{r}_3 + \vec{r}_2 \cdot \vec{r}_4 + \vec{r}_3 \cdot \vec{r}_4 + \vec{r}_2 \cdot \vec{r}_5 + \vec{r}_3 \cdot \vec{r}_5 + \vec{r}_4 \cdot \vec{r}_5) - D(\vec{r}_1 \cdot \vec{r}_2 + \vec{r}_1 \cdot \vec{r}_3 + \vec{r}_1 \cdot \vec{r}_4 + \vec{r}_1 \cdot \vec{r}_5)\right] \vec{r}_5 \cdot \left[\frac{1}{4}(\vec{r}_2 + \vec{r}_3 + \vec{r}_4 + \vec{r}_5) - \vec{r}_1\right] Y_1^{1*}(\Omega_5) Y_1^1(\Omega_{R_5}) \times d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

where

$$A = \frac{1}{2}\mu_1 \div \frac{3}{8}\alpha_1 \div \frac{\beta'}{40} \div \frac{\mu_1}{10} = \left\{ \begin{array}{l} 3.871512 \\ 3.896512 \end{array} \right\} \times 10^{25} \text{ cm}^{-2}$$

$$B = \frac{1}{2}\mu_1 \div \frac{2}{5}\beta' \div \frac{\mu_1}{10} = \left\{ \begin{array}{l} 3.091512 \\ 3.491512 \end{array} \right\} \times 10^{25} \text{ cm}^{-2}$$

$$C = \frac{1}{4}\alpha_1 \div \frac{\beta'}{20} \div \frac{\mu_1}{5} = \left\{ \begin{array}{l} 0.239496 \\ 0.189496 \end{array} \right\} \times 10^{25} \text{ cm}^{-2}$$

$$D = \frac{1}{5}(\mu, -\beta') = \left\{ \begin{array}{l} 0.28050h \\ 0.08050h \end{array} \right\} \times 10^{25} \text{cm}^{-2}.$$

The appearance of two values is due to the two possible values of the width parameter  $\beta'$ . Such pairs of values will appear throughout the calculation of the expansion coefficient of the ground state  $a_1$ . Using the method of App.I there results

$$\left\langle (12345)_1 \mid (1234;5) \right\rangle = \left\{ \begin{array}{l} 0.10156 \\ 0.09392 \end{array} \right\} \times 10^{-169} \text{cm}^{-1}h,$$

$$\left\langle (12345)_1 \mid (5234;1) \right\rangle = \left\{ \begin{array}{l} 0.2532h \\ 0.2412h \end{array} \right\} \times 10^{-170} \text{cm}^{-1}h.$$

Taking the normalization constants  $N_{\text{SML}}$  and  $N_{\text{CM}}$  from App.III, and substituting the above values into eq.(II-5) leads to

$$a_1 = \left\{ \begin{array}{l} 0.6268 \\ 0.6354 \end{array} \right\}.$$

Thus, the quantity  $|a_1|^2$  is

$$|a_1|^2 = \left\{ \begin{array}{l} 0.393 \\ 0.402 \end{array} \right\}.$$

(ii). The HOSM spatial wave function for the configuration  $(1s)^{-1}(2s)^1$  is

$$(12345)_2 = \exp\left(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2\right) \vec{r}_5 L_1^{\frac{1}{2}}(\mu_1 r_1^2) Y_1^1(\Omega_5),$$

where

$$L_1^{\frac{1}{2}}(\mu_1 r_1^2) = \frac{3}{2} \mu_1 r_1^2.$$

The exponential terms in the integrals  $\left\langle (12345)_2 \mid (1234;5) \right\rangle$

and  $\left\langle (12345)_2 \mid (5234;1) \right\rangle$  are the same as those in

$\left\langle (12345)_1 \mid (1234;5) \right\rangle$  and in  $\left\langle (12345)_1 \mid (5234;1) \right\rangle$  respectively.

However, one extra term (with  $\mu_1 r_1^2$ ) appears in the integrand,

so that, using the method outlined in App. II, there results

$$\langle (12345)_2 | (1234;5) \rangle = \begin{Bmatrix} 0.10587 \\ 0.09790 \end{Bmatrix} \times 10^{-169} \text{ cm}^{11},$$

$$\langle (12345)_2 | (5234;1) \rangle = \begin{Bmatrix} 0.02669 \\ 0.02543 \end{Bmatrix} \times 10^{-169} \text{ cm}^{11}.$$

Taking  $N_{SM2}$  and  $N_{CM}$  from App. III, and substitution of the above values into eq.(II-5) leads to

$$a_2 = \begin{Bmatrix} 0.3989 \\ 0.3947 \end{Bmatrix},$$

and

$$|a_2|^2 = \begin{Bmatrix} 0.159 \\ 0.156 \end{Bmatrix}.$$

(iii). The HOSM spatial wave function for the configuration  $(1s)^{-2}(1p)^2$  is

$$(12345)_3 = \exp(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2) |1\ 1\rangle_{523}$$

where

$$\begin{aligned} |1\ 1\rangle_{523} = & \frac{1}{\sqrt{2}} |1\ 1\rangle_5 |1\ 0\rangle_2 |1\ 0\rangle_3 - \frac{1}{\sqrt{6}} |1\ 0\rangle_5 |1\ 1\rangle_2 \\ & |1\ 0\rangle_3 - \frac{1}{3} |1\ 1\rangle_5 |1\ -1\rangle_2 |1\ 1\rangle_3 \\ & - \frac{1}{3} |1\ -1\rangle_5 |1\ 1\rangle_2 |1\ 1\rangle_3. \end{aligned}$$

This can also be written in the following explicit form:

$$\begin{aligned} (12345)_3 = & \exp(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2) (\vec{r}_2 \cdot \vec{r}_3) \vec{r}_5 \left[ \frac{1}{\sqrt{2}} Y_1^1(\Omega_5) Y_1^0(\Omega_2) Y_1^0(\Omega_3) \right. \\ & - \frac{1}{\sqrt{6}} Y_1^0(\Omega_5) Y_1^1(\Omega_2) Y_1^0(\Omega_3) - \frac{1}{3} Y_1^1(\Omega_5) Y_1^{-1}(\Omega_2) Y_1^1(\Omega_3) \\ & \left. - \frac{1}{3} Y_1^{-1}(\Omega_5) Y_1^1(\Omega_2) Y_1^1(\Omega_3) \right]. \end{aligned}$$

Again using the method of App. II,

$$\langle (12345)_3 | (1234;5) \rangle = \begin{Bmatrix} 0.01667 \\ 0.01542 \end{Bmatrix} \times 10^{-169} \text{ cm}^{14}$$

and

$$\langle (12345)_3 | (5234;1) \rangle = \begin{Bmatrix} 0.08528 \\ 0.07977 \end{Bmatrix} \times 10^{-170} \text{ cm}^{14}.$$

Substituting  $N_{SM3}$  and  $N_{CM}$  from App. III and the values of

$$\langle (12345)_3 | (1234;5) \rangle \text{ and } \langle (12345)_3 | (5234;1) \rangle \text{ into eq.(II-5)}$$

gives

$$a_3 = \begin{Bmatrix} 0.4592 \\ 0.4589 \end{Bmatrix},$$

and

$$|a_3|^2 = \begin{Bmatrix} 0.210 \\ 0.210 \end{Bmatrix}.$$

(iv). For the configuration  $(1p)^{-1}(2p)^1$ , the spatial wave function for the HOSM is

$$(12345)_4 = \exp\left(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2\right) \bar{r}_5 L_1^{3/2}(\mu_1 r_5^2) Y_1^1(\Omega_5)$$

where

$$L_1^{3/2}(\mu_1 r_5^2) = \frac{5}{2} \mu_1 r_5^2.$$

Using the method of App. II, there results

$$\langle (12345)_4 | (1234;5) \rangle = \begin{Bmatrix} 0.19105 \\ 0.18510 \end{Bmatrix} \times 10^{-169} \text{ cm}^{14}$$

and

$$\langle (12345)_4 | (5234;1) \rangle = \begin{Bmatrix} 0.04817 \\ 0.04792 \end{Bmatrix} \times 10^{-169} \text{ cm}^{14}.$$

Use of eq.(II-5) with the given  $N_{SM1}$ ,  $N_{CM}$  and the values of the integrals given above results in

$$a_4 = \begin{cases} 0.3527 \\ 0.3512 \end{cases}$$

and

$$|a_4|^2 = \begin{cases} 0.124 \\ 0.123 \end{cases}.$$

The states of Subsecs. (ii), (iii) and (iv) are those in the HOSM scheme having two quanta of excitation above the ground state configuration  $(1s)^4(1p)^1$ . In what follows, a calculation is made of the admixture amplitude for states having four quanta of excitation above the ground state configuration  $(1s)^4(1p)^1$ .

(v). If two nucleons have been excited from the 1s shell to the 2s shell each with two quanta of energy, then their configuration is  $(1s)^2(2s)^2$ . For this state, the HOSM spatial wave function is

$$(12345)_5 = \exp\left(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2\right) \bar{r}_5^{\frac{1}{2}} L_1^{\frac{1}{2}}(\mu_1 r_1^2) L_1^{\frac{1}{2}}(\mu_1 r_4^2) Y_1^1(\Omega_5)$$

where

$$L_1^{\frac{1}{2}}(\mu_1 r_1^2) = \frac{3}{2} - \mu_1 r_1^2, \quad L_1^{\frac{1}{2}}(\mu_1 r_4^2) = \frac{3}{2} - \mu_1 r_4^2.$$

By using the method in App. II as before, there results

$$\langle (12345)_5 | (12345) \rangle = \begin{cases} 0.10537 \\ 0.09750 \end{cases} \times 10^{-169} \text{ cm}^{-14}$$

and

$$\langle (12345)_5 | (5234;1) \rangle = \begin{Bmatrix} 0.02706 \\ 0.02578 \end{Bmatrix} \times 10^{-169} \text{ cm}^{14}.$$

Thus, from App. III, we have

$$a_5 = \begin{Bmatrix} 0.3075 \\ 0.3085 \end{Bmatrix}$$

and

$$|a_5|^2 = \begin{Bmatrix} 0.094 \\ 0.095 \end{Bmatrix}.$$

(vi). For the configuration  $(1s)^{-1}(3s)^1$ , the HOSM spatial wave function is

$$(12345)_6 = \exp\left(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2\right) F_5 L_2^{\frac{1}{2}}(\mu_1 r_1^2) Y_1^1(\Omega_5)$$

where

$$L_2^{\frac{1}{2}}(\mu_1 r_1^2) = \frac{15}{8} - \frac{5}{2} \mu_1 r_1^2 + \frac{1}{8} \mu_1^2 r_1^4.$$

Then applying the method in App. II gives

$$\langle (12345)_6 | (1234;5) \rangle = \begin{Bmatrix} 0.08488 \\ 0.07849 \end{Bmatrix} \times 10^{-169} \text{ cm}^{14}$$

and

$$\langle (12345)_6 | (5234;1) \rangle = \begin{Bmatrix} 0.02177 \\ 0.02074 \end{Bmatrix} \times 10^{-169} \text{ cm}^{14}.$$

Thus eq.(II-5) gives

$$a_6 = \begin{Bmatrix} 0.1161 \\ 0.1165 \end{Bmatrix}$$

and

$$|a_6|^2 = \left\{ \begin{array}{l} 0.013 \\ 0.013 \end{array} \right\}.$$

(vii). The amplitudes of the remaining configurations given in Sec. 1, namely,  $(1s)^{-1}(1d)^1$ ,  $(1s)^{-2}(2s)^1(1d)^1$ ,  $(1s)^{-1}(1p)^{-1}(2s)^1(2p)^1$ ,  $(1p)^{-1}(3p)^1$ ,  $(1s)^{-1}(2d)^1$  have been calculated, and were found to be small. The amplitudes  $|a_i|^2$  for these states are two or more orders of magnitude smaller than 0.01 (i.e., 1%), and so are negligible.

In order to check whether the above calculations satisfy the condition (I-9), the sum of the squares of the expansion coefficients is calculated; it is

$$\sum_{i=1}^6 |a_i|^2 = \left\{ \begin{array}{l} 0.993 \\ 0.999 \end{array} \right\}.$$

The sum rule is therefore satisfied to at least two significant figures.

CHAPTER III

Expansion of the Cluster Model Wave Function  
of the Second Excited State

1. The HOSM Scheme

The HOSM interprets the second excited state of  $\text{He}^5$  as three nucleons in the 1s shell and two nucleons in the 1p shell  $[(1s)^3(1p)^2, \text{ or } (1s)^{-1}(1p)^1 \text{ to the ground state}]$ . The total orbital angular momentum can therefore be  $L=2, 1$  or  $0$ . Since the second excited state of  $\text{He}^5$  has positive parity,  $L=1$  is inadmissible. On the other hand, if  $L=2$ , and since  $J=\frac{3}{2}$ , then the spin wave function must be orthogonal to that of the cluster model. This is because in the cluster model spin wave function  $S=\frac{3}{2}$ ; that is, four nucleons have spin "up" and one nucleon has spin "down", while the spin wave function of HOSM would have three nucleons with spin "down" and two nucleons with spin "up". Thus, only one choice remains, namely  $L=0$ . Then, as stated in Ch. I, the HOSM spin wave function is the same as that of the cluster model.

The configurations having three quanta of excitation and five quanta of excitation above the  $(1s)^4(1p)^1$  state, which have the same total angular momentum and parity as the second excited state ( $3/2^+$ ) are

Three quanta of excitation:

$$(1s)^{-2}(1p)^1(2s)^1, \quad (1s)^{-2}(1p)^1(1d)^1, \quad (1s)^{-1}(2p)^1;$$

Five quanta of excitation:

$$\begin{aligned} &(1s)^{-3}(1p)^1(2s)^2, & (1s)^{-3}(1p)^1(2s)^1(1d)^1, & (1s)^{-1}(1p)^{-1}(2p)^2, \\ &(1s)^{-2}(1p)^1(3s)^1, & (1s)^{-2}(2s)^1(2p)^1, & (1s)^{-2}(1d)^1(2p)^1, \\ &(1s)^{-2}(1p)^1(2d)^1. \end{aligned}$$

## 2. The General Formula for the Expansion Coefficients

The unantisymmetrized and antisymmetrized HOSM wave functions for the second excited state of  $He^5$  are

$$\phi_{SMi} = N_{SMi} (12345)_i \frac{1}{\sqrt{6}} [(\alpha_1 \beta_3 + \beta_1 \alpha_3) \alpha_2 - 2 \alpha_1 \beta_2 \alpha_3] \alpha_4 \alpha_5 \quad (III-1)$$

$$\begin{aligned} \mathcal{A} \phi_{SMi} = \frac{N_{SMi}}{4 \sqrt{6}} \{ &(\alpha_2 \beta_1 - \beta_2 \alpha_1) \alpha_3 \alpha_4 \alpha_5 [(12345)_i - (12435)_i] \\ &+ (\beta_2 \alpha_5 - \alpha_2 \beta_5) \alpha_1 \alpha_3 \alpha_4 [(52341)_i - (52431)_i] \\ &+ (\beta_5 \alpha_1 - \alpha_5 \beta_1) \alpha_2 \alpha_3 \alpha_4 [(15342)_i - (15432)_i] \}. \quad (III-2) \end{aligned}$$

The subscript  $i$  has the same meaning as stated in the previous chapter.

On the other hand, the unantisymmetrized and antisymmetrized cluster model wave functions for the second excited state of  $He^5$  are

$$\phi_{CM} = N_{CM} (123;45) \frac{1}{\sqrt{6}} [(\alpha_1 \beta_3 + \beta_1 \alpha_3) \alpha_2 - 2 \alpha_1 \beta_2 \alpha_3] \alpha_4 \alpha_5 \quad (III-3)$$

and

$$\phi_{CM} = \frac{N_{CM}}{4\sqrt{6}} \left\{ (\alpha_2 \beta_1 - \beta_2 \alpha_1) \alpha_3 \alpha_4 \alpha_5 \left[ (123;45) - (121;35) \right] \right. \\ \left. + (\beta_2 \alpha_5 - \alpha_2 \beta_5) \alpha_1 \alpha_3 \alpha_4 \left[ (523;41) - (524;31) \right] \right. \\ \left. + (\beta_5 \alpha_1 - \alpha_5 \beta_1) \alpha_2 \alpha_3 \alpha_4 \left[ (153;42) - (154;32) \right] \right\}. \quad (III-4)$$

The normalization constants for both model wave functions are determined by eq.(I-4) and the numerical values are given in the second part of App. III.

The expansion coefficient  $b_i$  is given by

$$b_i = \frac{N_{SMi} N_{CM}}{8} \left\{ \left\langle (12345)_i \mid (123;45) - 2(124;35) + (524;31) \right\rangle \right\}. \quad (III-5)$$

### 3. Numerical Calculation of the Expansion Coefficients

(i). The HOSM spatial wave function for the configuration

$(1s)^{-1}(1p)^1$  is

$$(12345)_1 = \exp\left(-\frac{1}{2}\mu\right) \sum_{i=1}^5 r_i^2 \vec{r}_i \cdot \vec{r}_5 \mid 0 \ 0 \rangle_{45}$$

where

$$\mid 0 \ 0 \rangle_{45} = \frac{1}{\sqrt{3}} \left[ Y_1^1(\Omega_4) Y_1^{-1}(\Omega_5) + Y_1^{-1}(\Omega_4) Y_1^1(\Omega_5) - Y_1^0(\Omega_4) Y_1^0(\Omega_5) \right].$$

Thus,

$$\left\langle (12345)_1 \mid (123;45) \right\rangle \\ = \int \exp\left\{ - \left[ A(r_1^2 + r_2^2 + r_3^2) + B(r_4^2 + r_5^2) + C(\vec{r}_1 \cdot \vec{r}_2 + \vec{r}_1 \cdot \vec{r}_3 + \vec{r}_2 \cdot \vec{r}_3) \right. \right. \\ \left. \left. + D(\vec{r}_1 \cdot \vec{r}_4 + \vec{r}_2 \cdot \vec{r}_4 + \vec{r}_3 \cdot \vec{r}_4 + \vec{r}_1 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_5 + \vec{r}_3 \cdot \vec{r}_5) + E\vec{r}_4 \cdot \vec{r}_5 \right] \right\} \vec{r}_4 \cdot \vec{r}_5 \\ \times \left[ \frac{1}{9}(r_1^2 + r_2^2 + r_3^2 + 2\vec{r}_1 \cdot \vec{r}_2 + 2\vec{r}_1 \cdot \vec{r}_3 + 2\vec{r}_2 \cdot \vec{r}_3) + \frac{1}{4}(r_4^2 + r_5^2 + 2\vec{r}_4 \cdot \vec{r}_5) \right. \\ \left. - \frac{1}{3}(\vec{r}_1 \cdot \vec{r}_4 + \vec{r}_2 \cdot \vec{r}_4 + \vec{r}_3 \cdot \vec{r}_4 + \vec{r}_1 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_5 + \vec{r}_3 \cdot \vec{r}_5) \right] d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5,$$

$$\langle (12345)_1 | (124;35) \rangle$$

$$= \int \exp \left\{ - \left[ A(r_1^2 + r_2^2 + r_4^2) + B(r_3^2 + r_5^2) + C(\vec{r}_1 \cdot \vec{r}_2 + \vec{r}_1 \cdot \vec{r}_4 + \vec{r}_2 \cdot \vec{r}_4) \right. \right. \\ \left. \left. + D(\vec{r}_1 \cdot \vec{r}_3 + \vec{r}_2 \cdot \vec{r}_3 + \vec{r}_3 \cdot \vec{r}_4 + \vec{r}_1 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_5 + \vec{r}_4 \cdot \vec{r}_5) + E\vec{r}_3 \cdot \vec{r}_5 \right] \right\} \vec{r}_4 \cdot \vec{r}_5 \\ \times \left[ \frac{1}{9}(r_1^2 + r_2^2 + r_4^2 + 2\vec{r}_1 \cdot \vec{r}_2 + 2\vec{r}_1 \cdot \vec{r}_4 + 2\vec{r}_2 \cdot \vec{r}_4) + \frac{1}{4}(r_3^2 + r_5^2 + 2\vec{r}_3 \cdot \vec{r}_5) \right. \\ \left. - \frac{1}{3}(\vec{r}_1 \cdot \vec{r}_3 + \vec{r}_2 \cdot \vec{r}_3 + \vec{r}_3 \cdot \vec{r}_4 + \vec{r}_1 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_5 + \vec{r}_4 \cdot \vec{r}_5) \right] d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

and

$$\langle (12345)_1 | (524;31) \rangle$$

$$= \int \exp \left\{ - \left[ A(r_5^2 + r_2^2 + r_4^2) + B(r_3^2 + r_1^2) + C(\vec{r}_2 \cdot \vec{r}_5 + \vec{r}_4 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_4) \right. \right. \\ \left. \left. + D(\vec{r}_3 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_3 + \vec{r}_3 \cdot \vec{r}_4 + \vec{r}_1 \cdot \vec{r}_5 + \vec{r}_1 \cdot \vec{r}_2 + \vec{r}_1 \cdot \vec{r}_4) + E\vec{r}_1 \cdot \vec{r}_3 \right] \right\} \vec{r}_4 \cdot \vec{r}_5 \\ \times \left[ \frac{1}{9}(r_2^2 + r_4^2 + r_5^2 + 2\vec{r}_2 \cdot \vec{r}_5 + 2\vec{r}_2 \cdot \vec{r}_4 + 2\vec{r}_4 \cdot \vec{r}_5) + \frac{1}{4}(r_1^2 + r_3^2 + 2\vec{r}_1 \cdot \vec{r}_3) \right. \\ \left. - \frac{1}{3}(\vec{r}_3 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_3 + \vec{r}_3 \cdot \vec{r}_4 + \vec{r}_1 \cdot \vec{r}_5 + \vec{r}_1 \cdot \vec{r}_2 + \vec{r}_1 \cdot \vec{r}_4) \right] d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5,$$

where

$$A = \frac{3}{5} \mu_1 + \frac{1}{3} \alpha + \frac{\beta}{15} = 3.212578 \times 10^{25} \text{ cm}^{-2}$$

$$B = \frac{3}{5} \mu_1 + \frac{1}{4} \bar{\alpha} + \frac{3}{20} \beta = 3.449812 \times 10^{25} \text{ cm}^{-2}$$

$$C = -\frac{1}{3} \alpha + \frac{2}{15} \beta + \frac{1}{5} \mu_1 = 0.037362 \times 10^{25} \text{ cm}^{-2}$$

$$D = \frac{1}{5} (\mu_1 - \beta) = 0.646104 \times 10^{25} \text{ cm}^{-2}$$

$$E = -\frac{1}{2} \bar{\alpha} + \frac{3}{10} \beta + \frac{1}{5} \mu_1 = -1.532896 \times 10^{25} \text{ cm}^{-2}$$

Here it should be pointed out that in the determination of

both normalization constants and also in the integrations of the type  $\langle (12345)_1 | (123;45) \rangle$  some common factors have been omitted; these will not affect the results because the same factors have been neglected in both numerators and denominators of the expansion coefficients.

By using the method of App. II, there results

$$\langle (12345)_1 | (123;45) \rangle = 0.23236 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_1 | (124;35) \rangle = -0.10674 \times 10^{-199} \text{ cm}^{16}$$

and

$$\langle (12345)_1 | (524;31) \rangle = 0.00074 \times 10^{-199} \text{ cm}^{16}.$$

Equation (III-5) then gives

$$b_1 = 0.5479$$

and

$$|b_1|^2 = 0.296.$$

(ii). The HOSM spatial wave function for the configuration

$(1s)^{-2}(1p)^1(2s)^1$  is

$$(12345)_2 = \exp(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2) L_1^{\frac{1}{2}}(\mu_1 r_1^2) \vec{r}_4 \cdot \vec{r}_5 | 0 \ 0 \rangle_{45}$$

where

$$L_1^{\frac{1}{2}}(\mu_1 r_1^2) = \frac{3}{2} - \mu_1 r_1^2.$$

Since the exponential term in the integrals are all the same, they need not be written down explicitly. An application of the method of App. II then gives

$$\langle (12345)_2 | (123;45) \rangle = 0.2068 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_2 | (124;35) \rangle = -0.09517 \times 10^{-199} \text{ cm}^{16}$$

and

$$\langle (12345)_2 | (524;31) \rangle = 0.00066 \times 10^{-199} \text{ cm}^{16},$$

so that

$$b_2 = 0.4013$$

and

$$|b_2|^2 = 0.161.$$

(iii). The HOSM spatial wave function for the configuration

$(1s)^{-2}(1p)^1(1d)^1$  is

$$(12345)_3 = \exp(-\frac{1}{2}M_i \sum_{i=1}^5 r_i^2) r_1^2 r_4 r_5 |0\ 0\rangle_{145}$$

where

$$\begin{aligned} |0\ 0\rangle_{145} = & \frac{1}{\sqrt{5}} \{ |1\ 1\rangle_4 |1\ 1\rangle_5 |2\ -2\rangle_1 \\ & + |1\ -1\rangle_4 |1\ -1\rangle_5 |2\ 2\rangle_1 - \frac{1}{\sqrt{2}} [ (|1\ 1\rangle_4 |1\ 0\rangle_5 \\ & + |1\ 0\rangle_4 |1\ 1\rangle_5) |2\ -1\rangle_1 + (|1\ -1\rangle_4 |1\ 0\rangle_5 \\ & + |1\ 0\rangle_4 |1\ -1\rangle_5) |2\ 1\rangle_1 ] \\ & + \frac{1}{\sqrt{6}} (|1\ 1\rangle_4 |1\ -1\rangle_5 + |1\ -1\rangle_4 |1\ 1\rangle_5) |2\ 0\rangle_1 \}. \end{aligned}$$

Again applying the method of App. II, there results

$$\langle (12345)_3 | (123;45) \rangle = 0.04597 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_3 | (124;35) \rangle = -0.02116 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_3 | (524;31) \rangle = 0.000146 \times 10^{-199} \text{ cm}^{16}.$$

Equation (III-5) gives finally

$$b_3 = 0.4950$$

and

$$|b_3|^2 = 0.245.$$

(iv). The HOSM spatial wave function for the configuration

$(1s)^{-1}(2p)^1$  is

$$(12345)_4 = \exp\left(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2\right) \vec{r}_4 \cdot \vec{r}_5 L_1^{3/2}(\mu_1 r_5^2) | 0 \ 0 \rangle_{45}$$

where

$$L_1^{3/2}(\mu_1 r_5^2) = \frac{5}{2} - \mu_1 r_5^2.$$

The method in App. II gives

$$\langle (12345)_4 | (123;45) \rangle = 0.31608 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_4 | (124;35) \rangle = -0.14546 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_4 | (524;31) \rangle = 0.0010 \times 10^{-199} \text{ cm}^{16}.$$

Again, from eq.(III-5), the expansion coefficient and its square

are

$$b_4 = 0.3541$$

$$|b_4|^2 = 0.125.$$

(v). The HOSM spatial wave function for the configuration  $(1s)^{-3}(1p)^1(2s)^2$  is

$$(12345)_5 = \exp(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2) L_1^{\frac{1}{2}}(\mu_1 r_1^2) L_1^{\frac{1}{2}}(\mu_1 r_2^2) | 0 0 \rangle_{45}$$

where

$$L_1^{\frac{1}{2}}(\mu_1 r_i^2) = \frac{3}{2} - \mu_1 r_i^2.$$

Using the same method as above gives

$$\langle (12345)_5 | (123;45) \rangle = 0.20969 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_5 | (124;35) \rangle = -0.09650 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_5 | (524;31) \rangle = 0.00066 \times 10^{-199} \text{ cm}^{16}.$$

and eq.(III-5) gives

$$b_5 = 0.3323$$

and

$$| b_5 |^2 = 0.110.$$

(vi). The HOSM spatial wave function for the configuration  $(1s)^{-3}(1p)^1(2s)^1(1d)^1$  is

$$(12345)_6 = \exp(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2) r_1^2 r_4^2 r_5^2 L_1^{\frac{1}{2}}(\mu_1 r_2^2) | 0 0 \rangle_{145}$$

where

$$L_1^{\frac{1}{2}}(\mu_1 r_2^2) = \frac{3}{2} - \mu_1 r_2^2,$$

and  $| 0 0 \rangle_{145}$  is given in (iii). Then the integrals are

$$\langle (12345)_6 | (123;45) \rangle = 0.02331 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_6 | (124;35) \rangle = -0.01073 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_6 | (524;31) \rangle = 0.00007 \times 10^{-199} \text{ cm}^{16},$$

so that,

$$b_6 = 0.2047$$

and

$$|b_6|^2 = 0.042.$$

(vii). The HOSM spatial wave function for the configuration  $(1s)^{-1}(1p)^{-1}(2p)^2$  is

$$(12345)_7 = \exp(-\frac{1}{2}\mu, \sum_{i=1}^5 r_i^2) \vec{r}_4 \cdot \vec{r}_5 L_1^{3/2}(\mu, r_5^2) L_1^{3/2}(\mu, r_4^2) | 0 \ 0 \rangle_{45}$$

where

$$L_1^{3/2}(\mu, r_i^2) = \frac{5}{2} - \mu, r_i^2.$$

Then the numerical values of the integrals are

$$\langle (12345)_7 | (123;45) \rangle = 0.30587 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_7 | (124;35) \rangle = -0.14076 \times 10^{-199} \text{ cm}^{16}$$

$$\langle (12345)_7 | (524;31) \rangle = 0.00097 \times 10^{-199} \text{ cm}^{16}.$$

Equation (III-5) gives then

$$b_7 = 0.127$$

and

$$|b_7|^2 = 0.016.$$

(viii). The amplitudes of the other configurations given in Sec.1 were also calculated, and found to be small. They are three or more orders of magnitude smaller than 0.01, and so are negligible.

On the other hand, there may be some contribution from the excitation of the two nucleons in the 1p level to the 2s level, with one quantum of excitation for each nucleon. Then, however the HOSM spatial wave function is completely symmetric and therefore cannot be antisymmetrized; thus, no contribution results.

The sum of the squares of the expansion coefficients (i.e., the intensities) is

$$\sum_{i=1}^7 |b_i|^2 = 0.999.$$

## CHAPTER IV

### Conclusion and Discussion

The HOSM describes the individual nucleons as moving in a common harmonic oscillator potential well. It is indeed a very simple and easily understandable model, but this simple model cannot describe details of nuclear structure very well. The reason for this of course is that the oscillator potential is not the real nuclear potential; in actual nuclei, the nuclear potential is more complicated than the oscillator potential. For instance, internucleon interactions must be accounted for in the actual nuclear potential, and these are not included in the HOSM potential. Thus, the HOSM eigenstates are not the eigenstates of the actual nuclear potential, and so the nuclear state wave functions cannot be simply replaced by the HOSM wave functions. If the oscillator potential is modified, then the nuclear state wave functions will be modified. As was mentioned in Ch. I, since the HOSM eigenfunctions are orthogonal to each other and span the whole configuration space, so the modified eigenfunctions can be expanded as a linear combination of the HOSM eigenfunctions. Thus, the modified eigenfunctions include not only the basic HOSM eigenfunctions, but also the higher excited eigenfunctions. This configuration mixing can also be calculated by the perturbation method. If the additional potential (or residual interaction) is taken as a perturbation,

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then the expansion coefficients may be determined by using the perturbation method (12).

The HOSM wave functions usually give energy levels which are too low compared to the experimental results. In order to have a more realistic model, the differences in energy between the actual nuclear levels and the HOSM predictions must be reduced somehow. This can be accomplished by mixing in HOSM states of higher energies. The amounts of these higher states included in the configuration mixing are given simply by the coefficients.

It will be shown in App. IV that the simple cluster model (in which all the width parameters are equal) is exactly equivalent to the HOSM after the wave functions have been antisymmetrized. However, the generalized cluster model (in which the width parameters are all different) used here for  $\text{He}^5$  includes higher HOSM configurations automatically simply by allowing the width parameters to differ from one another.

The cluster model wave functions for the ground state and the second excited state of  $\text{He}^5$  seem to be quite good, at least in some respects, as for example the energy levels and the E1 transition probability. The mixture of HOSM configurations in the cluster model wave function will show how  $\text{He}^5$  must be treated using the shell model in order to achieve results of similar quality.

Tables 2 and 3 summarize the results of Ch. II and Ch. III respectively for the intensities of the mixing of the

HOSM configurations in the cluster model wave functions in the ground and second excited states. From first order perturbation theory, it is expected that configurations having the same number of quanta of excitation should appear in roughly the same amounts. This found to be the case in the present calculation, with the one exception that the  $(2s)^2$  configurations in both the ground and second excited states have intensities of comparable magnitude to those of the two quantum excitations. This may partly be due to the L-S coupling scheme; since the nucleons with the same  $l$  have very similar HOSM wave functions, then, from perturbation theory, the matrix element between these states may be large even though the energy difference is not small.

It is also interesting to note that, as was mentioned in Ch. II, the  $1d$  level does not contribute very significantly to the ground state; however, it can be seen from Table 3 that the second excited state has a fairly large contribution from the  $1d$  level. From perturbation theory, the matrix element for the  $1d$  state should be quite small, but the energy difference is also small, so that the expansion coefficient may not be small. This rather large contribution from the  $1d$  level indicates that the energy of the actual nuclear state is quite near to that of the HOSM  $1d$  level.

Figs. 2 and 3 show that the configuration mixing is insensitive to variations of the cluster model width parameters for the ground state when one parameter is held constant at

Configuration	Intensity* (%)
$(1s)^4 (1p)^1$	{ 39.3 } { 40.2 }
$(1s)^{-1}(2s)^1$	{ 15.9 } { 15.6 }
$(1s)^{-2}(1p)^2$	{ 21.0 } { 21.0 }
$(1p)^{-1}(2p)^1$	{ 12.4 } { 12.3 }
$(1s)^{-2}(2s)^2$	{ 9.4 } { 9.5 }
$(1s)^{-1}(3s)^1$	{ 1.3 } { 1.3 }
Total	{ 99.3 } { 99.9 }

Table 2. The intensities of the different configurational states found in the ground state cluster model wave function with width parameters:  $\alpha_1 = 4.33 \times 10^{25} \text{ cm}^{-2}$ ,  $\beta' = \left\{ \begin{matrix} 2.25 \\ 3.25 \end{matrix} \right\} \times 10^{25} \text{ cm}^{-2}$  and  $\mu_1 = 3.65252 \times 10^{25} \text{ cm}^{-2}$ .

---

\* The two different intensities correspond to the two different values of the width parameter  $\beta'$  of the cluster model.

Configuration	Intensity (%)
$(1s)^{-1}(1p)^1$	30.0
$(1s)^{-2}(1p)^1(2s)^1$	16.1
$(1s)^{-2}(1p)^1(1d)^1$	24.5
$(1s)^{-1}(2p)^1$	12.5
$(1s)^{-3}(1p)^1(2s)^2$	11.0
$(1s)^{-3}(1p)^1(2s)^1(1d)^1$	4.2
$(1s)^{-1}(1p)^{-1}(2p)^2$	1.6
Total	99.9

Table 3. The intensities of the different configurational states found in the second excited state cluster model wave function with width parameters:  $\alpha = 2.81 \times 10^{25} \text{cm}^{-2}$ ,

$\bar{\alpha} = 4.78 \times 10^{25} \text{cm}^{-2}$ ,  $\beta = 0.422 \times 10^{25} \text{cm}^{-2}$  and  $\mu_1 = 3.65252 \times 10^{25} \text{cm}^{-2}$ .

Pearlstein's value and the other is varied. In Fig.1 of Pearlstein et al (2) curves (c) and (e) are quite flat near the minimum. This indicates that with a certain variation of the parameter  $\beta'$  around the minimum, the energy of the ground state does not change very much. It is therefore not surprising that the intensities of the configurations do not change appreciably when  $\beta'$  is varied. It was also mentioned in the same work (2) that the energy is insensitive to the

compressibility of the alpha particle. In other words, the energy of the ground state is insensitive to variations of the width parameter  $\alpha$ , when  $\beta'$  is held constant. Thus, it is also plausible that the mixture of the various HOSM configurations will also be insensitive to the variation of  $\alpha$ .

The ratio of the cluster model width parameters  $\beta'/\alpha = \left\{ \begin{array}{l} 0.52 \\ 0.75 \end{array} \right\} < 1$ ; this indicates that the alpha particle cluster and the neutron wave functions do not overlap greatly (13). Also, according to the shell model, closed shell structures usually remain energetically preferred even when the wave functions of the nucleons in closed shells overlap those of surrounding nucleons very strongly. Both of these points indicate that the ground state of  $\text{He}^5$  is favourable to formation of an alpha-neutron cluster structure. On the other hand, in the last paragraph, the insensitivity of the configuration mixing to the variation of one of the cluster model width parameters was seen. This suggests that certain collections of nucleons exist which are highly stable as free particles and are bound together to form the ground state of  $\text{He}^5$ --this is so because marked variations in the width parameters involved have very little affect on the binding energy and on the relative amounts of the various configurations which contribute to the state. From the possible choices of the clusters which are highly stable and bound, it may be induced that the most favourable one is the alpha

particle-neutron structure. Thus, the results indicating the insensitivity of the configuration mixing to the variation of one of the cluster model width parameters is consistent with the cluster representation of the ground state of  $\text{He}^5$ .

No variation of the cluster model width parameters of the second excited state has been performed. However the configuration mixing will probably be quite sensitive to the variation of any one of the three width parameters  $\alpha$ ,  $\bar{\alpha}$  and  $\beta$ . This can be seen from Figs. 3, 4 and 5 of Pearlstein et al (2), which show that if any one of the three cluster model width parameters are varied, a fairly large variation of the energy results.

Fig. 4 shows that for  $\alpha_1 = \mu_1$ , the configuration mixing is still insensitive to variation of the cluster model width parameter  $\beta'$  for the ground state except near the region of  $\beta' = \mu_1$ . The physical meaning of setting  $\alpha_1 = \mu_1$  is that the alpha particle is treated as a set of four individual nucleons without correlations. However, if  $\beta'$  is not equal to  $\mu_1$ , then the extra neutron has correlations with the four nucleons. When  $\beta' = \mu_1$ , the nucleon correlations are completely broken down; i.e., the antisymmetrized ground state cluster model wave function is completely equivalent to the HOSM wave function of the  $(1s)^4(1p)^1$  level. Mathematically, this will be shown in App. IV.

The same sort of diagram as shown in Fig. 4 will result if  $\beta' = \mu_1$  and  $\alpha_1$  is varied. This means that the two-body correlations between the alpha particle and neutron are first eliminated. If  $\alpha_1$  approaches  $\mu_1$ , then the nucleon correlations within the alpha particle become smaller and smaller. At  $\alpha_1 = \mu_1$ , the nucleon correlations are completely broken down as above, and the same thing will happen again-i.e., the antisymmetrized ground state cluster model wave function is equivalent to the HOSM wave function of the  $(1s)^4(1p)^1$  level.

Since configurations (i), (ii), (iv), (v) and (vii) can contribute to the E1 transition, then it is seen that the HOSM configuration (i) can only contribute partially to the E1 transition probability. Since the energy levels of the HOSM wave functions are equally spaced, then an estimate of the level width of the second excited state of  $\text{He}^5$  may be made on the HOSM as 0.006859 relative to level width according to the cluster model. This is consistent with the results of Tran Duc and Smith (3), who estimate the ratio

$$\frac{\Gamma_{\gamma}(\text{s.p.})}{\Gamma_{\gamma}(\text{cluster model})} = 1/(1.55 \times 10^2).$$

Since nuclear quadrupole moments are quite sensitive to admixtures of different configurations with the same angular momentum and parity (9), (14), it may be interesting to extend the present work to a quantitative discussion of the nuclear quadrupole moment of  $\text{He}^5$ . The cluster model wave function of

the ground state gives no quadrupole moment, because essentially no d-state admixture is present (9). However, as shown in Ch. III and Table 3, the second excited state does have a significant amount of d-state admixture, and so it may have a large quadrupole moment, although it cannot be measured directly at present.

APPENDIX I

Evaluation of Integrals of the Type

$$\int (\tilde{r}Br) e^{-\tilde{r}Ar} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

In most of the calculations in Ch. II, as well as in the calculation of the normalization constant of the ground state cluster model wave function, integrals of the type

$$\int (\tilde{r}Br) e^{-\tilde{r}Ar} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

must be evaluated, where A and B are 5x5 square matrices and r is a column matrix. Here the symbol "~" designates the transpose of a matrix.

A well known theorem in matrix algebra (15) states that "If  $\tilde{r}Ar$  and  $\tilde{r}Br$  are real quadratic forms and if  $\tilde{r}Ar$  is positive definite, there exists a real non-singular linear transformation  $r=Cz$  which carries  $\tilde{r}Br$  into  $\varphi_1 z_1^2 + \varphi_2 z_2^2 + \dots + \varphi_n z_n^2$  and  $\tilde{r}Ar$  into  $z_1^2 + z_2^2 + \dots + z_n^2$  where  $\varphi_1, \varphi_2, \dots, \varphi_n$  are the roots of  $|\varphi A - B| = 0$ ". This theorem is useful in transforming the integrands of the above type to a form which may be easily evaluated.

Let

$$I = \int (\tilde{r}Br) e^{-\tilde{r}Ar} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5 \quad (AI-1)$$

In order to evaluate this integral, first apply an orthogonal transformation  $O_1$  which diagonalizes  $\tilde{r}Ar$  (15). Then

$$I = \int (\tilde{O}_1 E O_1 r) e^{-\tilde{S}D_1 r} d\vec{s}_1 d\vec{s}_2 d\vec{s}_3 d\vec{s}_4 d\vec{s}_5$$

where  $s$  is the new coordinate system and  $D_1$  is the diagonal matrix. A second coordinate transformation:

$$\vec{t}_1 = \sqrt{\rho_1} \vec{s}_1, \quad \vec{t}_2 = \sqrt{\rho_2} \vec{s}_2, \quad \vec{t}_3 = \sqrt{\rho_3} \vec{s}_3, \quad \vec{t}_4 = \sqrt{\rho_4} \vec{s}_4, \quad \vec{t}_5 = \sqrt{\rho_5} \vec{s}_5,$$

(or it may write in the matrix form as  $s=Ht$  where

$H = \text{diag}(1/\sqrt{\rho_1}, 1/\sqrt{\rho_2}, 1/\sqrt{\rho_3}, 1/\sqrt{\rho_4}, 1/\sqrt{\rho_5})$ ) is now applied to the integral  $I$ . Here,  $\rho_1, \rho_2, \rho_3, \rho_4, \rho_5$  are the roots of the determinantal equation  $|A - \lambda I| = 0$ . This leads to

$$\begin{aligned} I &= \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} \int (\tilde{t} \tilde{H} \tilde{O}_1 \tilde{B} \tilde{O}_1 \tilde{H} t) e^{-\tilde{t} \tilde{H} D_1 \tilde{H} t} d\vec{t}_1 d\vec{t}_2 d\vec{t}_3 d\vec{t}_4 d\vec{t}_5 \\ &= \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} \int (\tilde{t} B_2 t) e^{-\tilde{t} I t} d\vec{t}_1 d\vec{t}_2 d\vec{t}_3 d\vec{t}_4 d\vec{t}_5 \end{aligned} \quad (\text{AI-2})$$

where  $B_2 = \tilde{H} \tilde{O}_1 \tilde{B} \tilde{O}_1 \tilde{H}$ . Finally, another orthogonal transformation  $O_2$  is applied to the integrand in order to diagonalize  $B_2$ . Thus,

$$\begin{aligned} I &= \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} \int (\tilde{z} \tilde{O}_2 \tilde{B}_2 \tilde{O}_2 z) e^{-\tilde{z} I z} d\vec{z}_1 d\vec{z}_2 d\vec{z}_3 d\vec{z}_4 d\vec{z}_5 \\ &= \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} \int (\tilde{z} D_2 z) e^{-\tilde{z} I z} d\vec{z}_1 d\vec{z}_2 d\vec{z}_3 d\vec{z}_4 d\vec{z}_5. \end{aligned} \quad (\text{AI-3})$$

This simplification comes about because  $O_2$  commutes with  $I$  and  $\tilde{O}_2 O_2 = I$ , so that this transformation does not affect the exponential term at all. Also, all transformations except  $H$  (or  $\vec{t}_i = \sqrt{\rho_i} \vec{s}_i$ ) are orthogonal transformations, and so their Jacobians  $|J| = 1$ . For the transformation  $H$ , the Jacobian is  $|J_H| = 1/(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}$ , and is already included in eq.(AI-2). Thus, eq.(AI-3) may be written explicitly in the following form

$$I = \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} \int \int \int \int \int_0^{\infty} (\varphi_1 z_1^2 + \varphi_2 z_2^2 + \dots + \varphi_5 z_5^2) \exp(-z_1^2 - z_2^2 - \dots - z_5^2) dz_1 dz_2 dz_3 dz_4 dz_5 \quad (AI-4)$$

where  $\varphi_1, \varphi_2, \dots, \varphi_5$  are the roots of the determinantal equation  $|B - \varphi A| = 0$ .

Since  $\rho_1, \rho_2, \dots, \rho_5$  are the roots of  $|A - \lambda I| = 0$ , then  $(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5) = \det A$ . Also, since the  $\varphi$ 's are the roots of  $|B - \varphi A| = 0$  (or  $|A^{-1}B - \varphi I| = 0$ ;  $A^{-1}$  exists because A is non-singular) then  $\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4 + \varphi_5 = \text{Trace}(A^{-1}B)$ .

Eq.(AI-4) can now be integrated as follows:

$$I = \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} \left[ (\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4 + \varphi_5) I_1 \right] \quad (AI-5)$$

where

$$I_1 = \int \int \int \int \int_0^{\infty} z_1^2 \exp(-z_1^2 - z_2^2 - z_3^2 - z_4^2 - z_5^2) dz_1 dz_2 dz_3 dz_4 dz_5.$$

$I_1$  is an elementary integral, and may be evaluated very easily.

In the calculation, an IBM subroutine program is used to evaluate  $A^{-1}$ . The same program determines  $(\det A^{-1})^{\frac{1}{2}} = 1/(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}$  and  $\text{Trace} A^{-1}B$ . In the program,  $SD = (\det A^{-1})^{\frac{1}{2}}$  and  $\text{Trace} = \text{Trace} A^{-1}B$ . In terms of these quantities eq.(AI-5) can be written as

$$I = SD \times \text{Trace} \times I_1.$$

The print-out sheet attached gives the program used for this purpose. Several remarks should be made concerning this program. As shown in the program, the final result is reached after the write statement of the trace. The rest of the

program is used to check the results. The first check is to determine whether or not  $A^{-1}A=I$  and  $B^{-1}B=I$ . Since  $B$  is usually singular,  $B^{-1}$  does not exist so in our program  $B^{-1}B$  is not unitary. If  $B$  is non-singular, however, we can form  $B^{-1}A$ , and the second check is to find the inverse of  $B^{-1}A$ , which should be equal to  $A^{-1}B$ . The second check was performed several times and it did indicate that the subroutine is very good.

In the above-mentioned method the exponential term was first diagonalized. On the other hand, if  $B$  is non-singular, the same method can be used, except that  $B$  is diagonalized first. It can be shown mathematically that these two different approaches are strictly equivalent. This is confirmed in the computations.

```

S.0001      C      MAIN PROBLEM
              DIMENSION A(25),B(25),C(5,5),E(5,5),F(5,5),G(5,5),H(5,5),P(5,5),
              IR(5,5),T(5,5),U(25),W(5,5),L(5),M(5)
S.0002      IJK=0
S.0003      600 READ (1,450) IPARAM
S.0004      450 FORMAT (I4)
S.0005      WRITE (3,451) IPARAM
S.0006      451 FORMAT (1H1,I4//)
S.0007      500 READ (1,3) (A(I),I=1,25),(B(I),I=1,25)
S.0008      3  FORMAT (5F14.8)

      C
      C      RETAIN A
      C
S.0009      DO 40 J=1,5
S.0010      G(J,1)=A(J)
S.0011      G(J,2)=A(J+5)
S.0012      G(J,3)=A(J+10)
S.0013      G(J,4)=A(J+15)
S.0014      40 G(J,5)=A(J+20)
S.0015      WRITE (3,41) ((G(I,J),I=1,5),J=1,5)
S.0016      41 FORMAT (1X,'G=',5X,5F14.8//)

      C
      C      RETAIN B
      C
S.0017      DO 20 J=1,5
S.0018      E(J,1)=B(J)
S.0019      E(J,2)=B(J+5)
S.0020      E(J,3)=B(J+10)
S.0021      E(J,4)=B(J+15)
S.0022      20 E(J,5)=B(J+20)
S.0023      WRITE (3,8) ((E(I,J),I=1,5),J=1,5)
S.0024      8  FORMAT (1X,'E=',5X,5F14.8//)

      C
      C      MAIN MATRIX INVERSION
      C
      C      WRITE OUT A INVERSE
      C
S.0025      N=5
S.0026      CALL MINV (A,N,D,L,M)
S.0027      DO 25 J=1,5
S.0028      F(J,1)=A(J)
S.0029      F(J,2)=A(J+5)
S.0030      F(J,3)=A(J+10)
S.0031      F(J,4)=A(J+15)
S.0032      25 F(J,5)=A(J+20)
S.0033      WRITE (3,10) ((F(I,J),I=1,5),J=1,5)
S.0034      10 FORMAT (1X,'F=',5X,5F14.8//)
S.0035      SD=SQRT(ABS(D))
S.0036      WRITE (3,14) D,SD
S.0037      14 FORMAT (1X,'D=',5X,F14.8,10X,'SD=',5X,F14.8//)

      C
      C      WRITE OUT B INVERSE
      C

```

```

C
S.0038 CALL MINV (B,N,D,L,M)
S.0039 DO 50 J=1,5
S.0040 H(J,1)=B(J)
S.0041 H(J,2)=B(J+5)
S.0042 H(J,3)=B(J+10)
S.0043 H(J,4)=B(J+15)
S.0044 50 H(J,5)=B(J+20)
S.0045 WRITE (3,51) ((H(I,J),I=1,5),J=1,5)
S.0046 51 FORMAT (1X,'H=',5X,5F14.8//)
S.0047 WRITE (3,15) D
S.0048 15 FORMAT (1X,'D=',5X,F14.8//)

```

```

C
C C EQUAL TO A INVERSE MULTIPLE B
C
S.0049 DO 1 I=1,5
S.0050 DO 1 J=1,5
S.0051 SUM=0.
S.0052 DO 2 K=1,5
S.0053 SUM=F(I,K)*F(K,J)+SUM
S.0054 2 CONTINUE
S.0055 C(I,J)=SUM
S.0056 1 CONTINUE
S.0057 WRITE (3,5) ((C(I,J),I=1,5),J=1,5)
S.0058 5 FORMAT (1X,'C=',5X,5F14.8//)
S.0059 SUM=0.
S.0060 DO 30 I=1,5
S.0061 SUM=C(I,I)+SUM
S.0062 TRACE=SUM
S.0063 30 CONTINUE
S.0064 WRITE (3,70) TRACE
S.0065 70 FORMAT (1X,'TRACE=',5X,F14.8//)

```

```

C
C CHECK WHETHER IT IS IDENTITY FOR A
C
S.0066 DO 101 I=1,5
S.0067 DO 101 J=1,5
S.0068 SUM=0.
S.0069 DO 102 K=1,5
S.0070 SUM=F(I,K)*G(K,J)+SUM
S.0071 102 CONTINUE
S.0072 P(I,J)=SUM
S.0073 101 CONTINUE
S.0074 WRITE (3,105) ((P(I,J),I=1,5),J=1,5)
S.0075 105 FORMAT (1X,'P=',5X,5F14.8//)

```

```

C
C CHECK WHETHER IT IS IDENTITY FOR B
C
S.0076 DO 111 I=1,5
S.0077 DO 111 J=1,5
S.0078 SUM=0.
S.0079 DO 112 K=1,5
S.0080 SUM=H(I,K)*E(K,J)+SUM
S.0081 112 CONTINUE

```

```

S.0082      R(I,J)=SUM
S.0083      111 CONTINUE
S.0084      WRITE (3,125) ((R(I,J),I=1,5),J=1,5)
S.0085      125 FORMAT (1X,'R=',5X,5F14.8//)
C
C
C          DOUBLE CHECK
C
C          T EQUAL TO B INVERSE MULTIPLE TO A
S.0086      DO 201 I=1,5
S.0087      DO 201 J=1,5
S.0088      SUM=0.
S.0089      DO 202 K=1,5
S.0090      SUM=H(I,K)*G(K,J)+SUM
S.0091      202 CONTINUE
S.0092      T(I,J)=SUM
S.0093      201 CONTINUE
S.0094      WRITE (3,205) ((T(I,J),I=1,5),J=1,5)
S.0095      205 FORMAT (1X,'T=',5X,5F14.8//)
C
C
C          FORMING U
S.0096      DO 300 J=1,5
S.0097      U(J)=T(J,1)
S.0098      U(J+5)=T(J,2)
S.0099      U(J+10)=T(J,3)
S.0100      U(J+15)=T(J,4)
S.0101      300 U(J+20)=T(J,5)
S.0102      CALL MINV (U,N,D,L,M)
C
C
C          WRITE OUT T INVERSE
S.0103      DO 400 J=1,5
S.0104      W(J,1)=U(J)
S.0105      W(J,2)=U(J+5)
S.0106      W(J,3)=U(J+10)
S.0107      W(J,4)=U(J+15)
S.0108      400 W(J,5)=U(J+20)
S.0109      WRITE (3,303) ((W(I,J),I=1,5),J=1,5)
S.0110      303 FORMAT (1X,'W=',5X,5F14.8)
S.0111      IJK=IJK+1
S.0112      IF (IJK-80)600,401,401
S.0113      401 CONTINUE
S.0114      RETURN
S.0115      END

```

SIZE OF COMMON 000000 PROGRAM 004832

END OF COMPILATION MAIN



C  
C

## SEARCH FOR LARGEST ELEMENT

S.0003 D=1.0  
S.0004 NK=-N  
S.0005 DO 80 K=1,N  
S.0006 NK=NK&N  
S.0007 L(K)=K  
S.0008 M(K)=K  
S.0009 KK=NK&K  
S.0010 BIGA=A(KK)  
S.0011 DO 20 J=K,N  
S.0012 IZ=N\*(J-1)  
S.0013 DO 20 I=K,N  
S.0014 IJ=IZ&I  
S.0015 10 IF(ABS(BIGA)-ABS(A(IJ)))15,20,20  
S.0016 15 BIGA=A(IJ)  
S.0017 L(K)=I  
S.0018 M(K)=J  
S.0019 20 CONTINUE

C  
C  
C

## INTERCHANGE ROWS

S.0020 J=L(K)  
S.0021 IF(J-K) 35,35,25  
S.0022 25 KI=K-N  
S.0023 DO 30 I=1,N  
S.0024 KI=KI&N  
S.0025 HOLD=-A(KI)  
S.0026 JI=KI-K&J  
S.0027 A(KI)=A(JI)  
S.0028 30 A(JI)=HOLD

C  
C  
C

## INTERCHANGE COLUMNS

S.0029 35 I=M(K)  
S.0030 IF(I-K) 45,45,38  
S.0031 38 JP=N\*(I-1)  
S.0032 DO 40 J=1,N  
S.0033 JK=NK&J  
S.0034 JI=JP&J  
S.0035 HOLD=-A(JK)  
S.0036 A(JK)=A(JI)  
S.0037 40 A(JI)=HOLD

C  
C  
C  
CDIVIDE COLUMN BY MINUS PIVOT (VALUE OF PIVOT ELEMENT IS  
CONTAINED IN BIGA)

S.0038 45 IF(BIGA) 48,46,48  
S.0039 46 D=0.0  
S.0040 RETURN  
S.0041 48 DO 55 I=1,N  
S.0042 IF(I-K) 50,55,50  
S.0043 50 IK=NK&I  
S.0044 A(IK)=A(IK)/(-BIGA)  
S.0045 55 CONTINUE

C  
C  
C

## REDUCE MATRIX

```
S.0046      DO 65 I=1,N
S.0047      IK=NK&I
S.0048      IJ=Y-N
S.0049      DO 65 J=1,N
S.0050      IJ=IJ&N
S.0051      IF(I-K) 60,65,60
S.0052      60 IF(J-K) 62,65,62
S.0053      62 KJ=IJ-I&K
S.0054      A(IJ)=A(IK)*A(KJ)&A(IJ)
S.0055      65 CONTINUE
```

C  
C  
C

## DIVIDE ROW BY PIVOT

```
S.0056      KJ=K-N
S.0057      DO 75 J=1,N
S.0058      KJ=KJ&N
S.0059      IF(J-K) 70,75,70
S.0060      70 A(KJ)=A(KJ)/BIGA
S.0061      75 CONTINUE
```

C  
C  
C

## PRODUCT OF PIVOTS

```
S.0062      D=D*BIGA
```

C  
C  
C

## REPLACE PIVOT BY RECIPROCAL

```
S.0063      A(KK)=1.07/BIGA
S.0064      80 CONTINUE
```

C  
C  
C

## FINAL ROW AND COLUMN INTERCHANGE

```
S.0065      K=N
S.0066      100 K=(K-1)
S.0067      IF(K) 150,150,105
S.0068      105 I=L(K)
S.0069      IF(I-K) 120,120,108
S.0070      108 JQ=N*(K-1)
S.0071      JR=N*(I-1)
S.0072      DO 110 J=1,N
S.0073      JK=JQ&J
S.0074      HOLD=A(JK)
S.0075      JI=JR&J
S.0076      A(JK)=-A(JI)
S.0077      110 A(JI)=HOLD
S.0078      120 J=M(K)
S.0079      IF(J-K) 100,100,125
S.0080      125 KI=K-N
S.0081      DO 130 I=1,N
S.0082      KI=KI&N
S.0083      HOLD=A(KI)
S.0084      JI=KI-K&J
S.0085      A(KI)=-A(JI)
```

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S.CC86 130 A(JI) =HOLD  
S.CC87 GO TO 100  
S.CC88 150 RETURN  
S.CC89 END

SIZE OF COMMON 000000 PROGRAM 002134  
END OF COMPILATION MINV

APPENDIX II

Evaluation of Integrals of the Type

$$\int (\tilde{r}Br)(\tilde{r}Cr)e^{-\tilde{r}Ar} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5$$

This type of integral is not as simple as the one dealt with in App. I. However, it may be somewhat simplified by using the same method as in App.I.

Let

$$I' = \int (\tilde{r}Br)(\tilde{r}Cr)e^{-\tilde{r}Ar} d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 d\vec{r}_5. \quad (AII-1)$$

An orthogonal transformation  $O_1$  is first applied to diagonalize  $A$ , and then  $H = \text{diag}(1/\sqrt{P_1}, 1/\sqrt{P_2}, 1/\sqrt{P_3}, 1/\sqrt{P_4}, 1/\sqrt{P_5})$  is used to get  $\tilde{z}Iz$  in the exponential term, as in App.I. Thus

$$\begin{aligned} I'' &= \int (\tilde{s}O_1 B O_1 s)(\tilde{s}O_1 C O_1 s)e^{-\tilde{s}D_1 s} ds_1 ds_2 ds_3 ds_4 ds_5 \\ &= \frac{1}{(P_1 P_2 P_3 P_4 P_5)^{\frac{1}{2}}} \int (\tilde{t}H O_1 B O_1 H t)(\tilde{t}H O_1 C O_1 H t)e^{-\tilde{t}I t} dt_1 dt_2 dt_3 dt_4 dt_5 \\ &= \frac{1}{(P_1 P_2 P_3 P_4 P_5)^{\frac{1}{2}}} \int (\tilde{t}B_2 t)(\tilde{t}C_2 t)e^{-\tilde{t}I t} dt_1 dt_2 dt_3 dt_4 dt_5 \end{aligned} \quad (AII-2)$$

where  $B_2 = \tilde{H}O_1 B O_1 H$  and  $C_2 = \tilde{H}O_1 C O_1 H$ . Another orthogonal transformation  $O_2$  can then be applied to diagonalize  $B_2$  or  $C_2$ , (depending on which will be more effective). That is, if  $B_2$  is more complicated than  $C_2$ , then it is diagonalized rather than  $C_2$ .

Assume for definiteness that  $B_2$  is to be diagonalized; then from eq. (AII-2)

$$I' = \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} \int (\tilde{u} \tilde{O}_2 u) (\tilde{u} \tilde{O}_2^* \tilde{O}_2 u) e^{-\tilde{u} \tilde{I} u} d\vec{u}_1 d\vec{u}_2 d\vec{u}_3 d\vec{u}_4 d\vec{u}_5$$

$$= \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} \int (\varphi_1 u_1^2 + \varphi_2 u_2^2 + \dots + \varphi_5 u_5^2) (\tilde{u} \tilde{C}_3 u) e^{-\tilde{u} \tilde{I} u} d\vec{u}_1 d\vec{u}_2 d\vec{u}_3 d\vec{u}_4 d\vec{u}_5$$

(AII-3)

where  $\tilde{C}_3 = \tilde{O}_2^* \tilde{C}_2 \tilde{O}_2$ , and  $(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5) = \det A$ . Thus,

$$I' = \frac{1}{(\rho_1 \rho_2 \rho_3 \rho_4 \rho_5)^{\frac{1}{2}}} (\varphi_1 I_1 + \varphi_2 I_2 + \varphi_3 I_3 + \varphi_4 I_4 + \varphi_5 I_5)$$

(AII-4)

where

$$I_i = \int u_i^2 (\tilde{u} \tilde{C}_3 u) e^{-\tilde{u} \tilde{I} u} d\vec{u}_1 d\vec{u}_2 d\vec{u}_3 d\vec{u}_4 d\vec{u}_5 \quad (i=1,2,3,4,5).$$

(AII-4')

In order to evaluate  $I'$  a different program from that used in App. I must be employed; since  $\tilde{O}_1$ , the  $\rho$ 's,  $H$ ,  $\tilde{O}_2$  and the  $\varphi$ 's must be determined, an IBM subroutine program to find the eigenvalues and eigenvectors of  $A$  and  $B_2$  is employed. The diagonalization of  $A$  gives the  $\rho$ 's,  $H$  and  $\tilde{O}_1^*$ ;  $B_2$  and  $\tilde{C}_2$  may be evaluated by using another short program. Then we can feed  $B_2$  to the same program to find its eigenvalues and eigenvectors. This determines the  $\varphi$ 's and  $\tilde{O}_2$ , and thereby  $\tilde{C}_3$ . Since the quadratic form  $(\tilde{u} \tilde{C}_3 u)$  is not a scalar, it must be borne in mind that all the cross terms are actually scalar products of two vectors, e.g.,  $\vec{r}_1 \cdot \vec{r}_2$ ,  $\vec{r}_3 \cdot \vec{r}_5$ , and so on. Thus before carrying out the integrations  $I_i$  in eq. (AII-4'), the integrations over angles must first be evaluated. When this is

---

\* The transformation matrix  $T$  of the program has been checked and is indeed an orthogonal transformation matrix, i.e.,  $\tilde{T}T=I$ .

done, the quadratic form  $\tilde{u}C_3u$  becomes  $\tilde{u}C_4u$  (where  $C_4$  is a matrix representation of the scalar quadratic form), and eq.(AII-4) becomes eq.(AII-4') becomes

$$I_i = \int u_i^2 (\tilde{u}C_4u) e^{-\tilde{u}Tu} du_1 du_2 du_3 du_4 du_5. \quad (\text{AII-4}''')$$

The Gauss-Laguerre method (16) is now applied in order to get the numerical values of the  $I_i$ . The integral  $I'$  can now be evaluated using eq.(AII-4) and these results, i.e., the  $\rho$ 's, the  $\varphi$ 's and  $I_i$ .

It may seem quite unreasonable at first sight to calculate  $I'$  by the above method: why not apply the Gauss-Laguerre method at the beginning? The reason for this is that experience has shown that if the integrand is complicated, then the accuracy of the result is poor. The situation is improved considerably when the integrand is first simplified, as was done above.

If more than three quadratic forms occur in the integrand, the same method of diagonalizing two of them may be used: one is the exponential term and the other is chosen for convenience. Thus,  $I$  is given by eq.(AII-4), with the  $I_i$  in the following form

$$I_i = \int u_i^2 (\tilde{u}C_3u) (\tilde{u}E_3u) e^{-\tilde{u}Tu} du_1 du_2 du_3 du_4 du_5.$$

It sometimes occurs that after diagonalization of  $A$  and eq.(AII-2) has been obtained, the remaining factors  $B_2$  and  $C_2$  are perfect squares. That is to say,  $\tilde{t}B_2t = (\tilde{t}L_1)(L_1t)$  and

$\tilde{t}C_2 t = (\tilde{t}L_2)(L_2 t)$ . Then the product  $(\tilde{t}L_1)(L_2 t)$  is a quadratic form, and eq.(AII-2) becomes

$$I = \frac{1}{(\beta_1 \beta_2 \beta_3 \beta_4 \beta_5)^{\frac{1}{2}}} \int (\tilde{t}Kt)(\tilde{t}Kt) e^{-\tilde{t}It} d\vec{t}_1 d\vec{t}_2 d\vec{t}_3 d\vec{t}_4 d\vec{t}_5$$

where  $K = \tilde{L}_1 L_2$ . A single orthogonal transformation can then be used to diagonalize the two resulting quadratic forms. This simplifies the calculation and gives the result up to five significant figures. Although this situation does not occur in all cases it nevertheless does arise in our calculation several times. This is useful in checking the results of the Gauss-Laguerre method.

In our programming for  $I_1$  of eq.(AII-4<sup>u</sup>), an IBM library program for the Gauss-Laguerre method and its data sets are used. However, it was not possible to run for 32 points (or roots) because about 25 minutes are then required for each run. Instead 15 points are used in this computation; this gives three to four significant figures, and is quite satisfactory for the present purpose.

The program for evaluating the eigenvalues and eigenvectors is attached.

APPENDIX III

Normalization Constants

The numerical calculation of the normalization constants

LEVEL 1 JUL 66

IBM OS/360 BASIC FORTRAN IV (E) COMPILATION

```

C      JACOBI ROTATIONS METHOD
C      FOR EIGENVALUES AND EIGENVECTORS
S.C001  DIMENSION A(100),R(100),S(10),D(10)
S.C002  600 READ (1,450) IPARAM
S.C003  450 FORMAT (I3)
S.C004  WRITE (3,451) IPARAM
S.C005  451 FORMAT (1H1,I3//)
S.C006  10 READ (1,50) MV
S.C007  WRITE(3,100)
S.C008  CALL MATIN(ICODA,A,100,NA,MA,ISA,IER)
S.C009  CALL MXOUT(ICODA,A,NA,MA,ISA,60,132,2)
S.C010  CALL EIGEN(A,R,NA,MV)
S.C011  DO 260 I=1,NA
S.C012  L=I&(I#I-1)/2
S.C013  260 S(I)=A(L)
S.C014  WRITE(3,180)(J,S(J),J=1,NA)
S.C015  WRITE(3,200)
S.C016  L=0
S.C017  DO 150 J=1,NA
S.C018  DO 160 I=1,NA
S.C019  L=L&1
S.C020  160 D(I)=R(L)
S.C021  150 WRITE(3,9)J,(D(I),I=1,NA)
S.C022  50 FORMAT(I10)
S.C023  9 FORMAT(7HOVECTOR,I3/7E16.8)
S.C024  180 FORMAT (/9X,14HEIGENVALUE NO.,I2,2H =,E16.8)
S.C025  200 FORMAT (/9X,11HEIGENVECTOR )
S.C026  100 FORMAT (/11X,24HJACOBI ROTATIONS METHOD /,
19X,33HFOR EIGENVALUES AND EIGENVECTORS./)
S.C027  GO TO 600
S.C028  END

```

SIZE OF COMMON 000000 PROGRAM 002124

END OF COMPILATION MAIN

LEVELC 1JUL66

IBM OS/360 BASIC FORTRAN IV (E) COMPILATION

```
C      JACOBI ROTATIONS METHOD
C      FOR EIGENVALUES AND EIGENVECTORS
S.C001      DIMENSION A(100),R(100),S(10),D(10)
S.C002      600 READ (1,450) IPARAM
S.C003      450 FORMAT (I3)
S.C004      WRITE (3,451) IPARAM
S.C005      451 FORMAT (1H1,I3///)
S.C006      10 READ (1,50) MV
S.C007      WRITE(3,100)
S.C008      CALL MATIN(ICODA,A,100,NA,MA,ISA,IER)
S.C009      CALL MXOUT(ICODA,A,NA,MA,ISA,60,132,2)
S.C010      CALL EIGEN(A,R,NA,MV)
S.C011      DO 260 I=1,NA
S.C012      L=I*(I-1)/2
S.C013      260 S(I)=A(L)
S.C014      WRITE(3,180)(J,S(J),J=1,NA)
S.C015      WRITE(3,200)
S.C016      L=0
S.C017      DO 150 J=1,NA
S.C018      DO 160 I=1,NA
S.C019      L=L&1
S.C020      160 D(I)=R(L)
S.C021      150 WRITE(3,9)J,(D(I),I=1,NA)
S.C022      50 FORMAT(I10)
S.C023      9 FORMAT(7HOVECTOR,I3/7E16.8)
S.C024      180 FORMAT (/9X,14HEIGENVALUE NO.,I2,2H =,E16.8)
S.C025      200 FORMAT (/9X,11HEIGENVECTOR )
S.C026      100 FORMAT (/11X,24HJACOBI ROTATIONS METHOD /,
19X,33HFOR EIGENVALUES AND EIGENVECTORS./)
S.C027      GO TO 600
S.C028      END
```

SIZE OF COMMON 000000 PROGRAM 002124

END OF COMPILATION MAIN

LEVEL 1JUL66

IBM OS/360 BASIC FORTRAN IV (E) COMPILATION

.....  
SUBROUTINE EIGEN

PURPOSE  
COMPUTE EIGENVALUES AND EIGENVECTORS OF A REAL SYMMETRIC  
MATRIX

USAGE  
CALL EIGEN(A,R,N,MV)

DESCRIPTION OF PARAMETERS

- A - ORIGINAL MATRIX (SYMMETRIC), DESTROYED IN COMPUTATION. RESULTANT EIGENVALUES ARE DEVELOPED IN DIAGONAL OF MATRIX A IN DESCENDING ORDER.
- R - RESULTANT MATRIX OF EIGENVECTORS (STORED COLUMNWISE, IN SAME SEQUENCE AS EIGENVALUES)
- N - ORDER OF MATRICES A AND R
- MV- INPUT CODE
  - 0 COMPUTE EIGENVALUES AND EIGENVECTORS
  - 1 COMPUTE EIGENVALUES ONLY (R NEED NOT BE DIMENSIONED BUT MUST STILL APPEAR IN CALLING SEQUENCE)

REMARKS  
ORIGINAL MATRIX A MUST BE REAL SYMMETRIC (STORAGE MODE=1)  
MATRIX A CANNOT BE IN THE SAME LOCATION AS MATRIX R

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED  
NONE

METHOD

DIAGONALIZATION METHOD ORIGINATED BY JACobi AND ADAPTED BY VON NEUMANN FOR LARGE COMPUTERS AS FOUND IN "MATHEMATICAL METHODS FOR DIGITAL COMPUTERS", EDITED BY A. RALSTON AND H.S. WILF, JOHN WILEY AND SONS, NEW YORK, 1962, CHAPTER 7

S.CCC1  
S.CCC2

SUBROUTINE EIGEN(A,R,N,MV)  
DIMENSION A(1),R(1)

.....  
IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE  
C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION  
STATEMENT WHICH FOLLOWS.

DOUBLE PRECISION A,R,ANORM,ANRMX,THR,X,Y,SINX,SINX2,COSX,  
COSX2,SINCS



```

S.0036      68 Y=-A(LM)/ SQRT(A(LM)*A(LM)&X*X)
S.0037      IF(X) 70,75,75
S.0038      70 Y=-Y
S.0039      75 SINX=Y/ SQRT(2.0*(1.0&( SQRT(1.0-Y*Y))))
S.0040      SINX2=SINX*SINX
S.0041      78 COSX= SQRT(1.0-SINX2)
S.0042      COSX2=COSX*COSX
S.0043      SINCS =SINX*COSX

```

C  
C  
C

ROTATE L AND M COLUMNS

```

S.0044      ILQ=N*(L-1)
S.0045      IMQ=N*(M-1)
S.0046      DO 125 I=1,N
S.0047      IQ=(I*I-1)/2
S.0048      IF(I-L) 80,115,80
S.0049      80 IF(I-M) 85,115,90
S.0050      85 IM=I&MQ
S.0051      GO TO 95
S.0052      90 IM=M&IQ
S.0053      95 IF(I-L) 100,105,105
S.0054      100 IL=I&LQ
S.0055      GO TO 110
S.0056      105 IL=L&IQ
S.0057      110 X=A(IL)*COSX-A(IM)*SINX
S.0058      A(IM)=A(IL)*SINX&A(IM)*COSX
S.0059      A(IL)=X
S.0060      115 IF(MV-1) 120,125,120
S.0061      120 ILR=IL&I
S.0062      IMR=IM&I
S.0063      X=R(ILR)*COSX-R(IMR)*SINX
S.0064      R(IMR)=R(ILR)*SINX&R(IMR)*COSX
S.0065      R(ILR)=X
S.0066      125 CONTINUE
S.0067      X=2.0*A(LM)*SINCS
S.0068      Y=A(LL)*COSX2&A(MM)*SINX2-X
S.0069      X=A(LL)*SINX2&A(MM)*COSX2&X
S.0070      A(LM)=(A(LL)-A(MM))*SINCS&A(LM)*(1.0&X2-SINX2)
S.0071      A(LL)=Y
S.0072      A(MM)=X

```

C  
C  
C  
C

TESTS FOR COMPLETION

TEST FOR M = LAST COLUMN

```

S.0073      130 IF(M=N) 135,140,135
S.0074      135 M=M&I
S.0075      GO TO 60

```

C  
C

TEST FOR L = SECOND FROM LAST COLUMN

```

S.0076      140 IF(L=N-1) 145,150,145
S.0077      145 L=L&I
S.0078      GO TO 55
S.0079      150 IF(L=N-1) 145,150,150

```

```

S.C080      155 IND=0
S.C081      GO TO 50
C
C          COMPARE THRESHOLD WITH FINAL NORM
S.C082      160 IF(THR-ANRMX) 165,165,45
C
C          SORT EIGENVALUES AND EIGENVECTORS
S.C083      165 IQ=-N
S.C084      DO 185 I=1,N
S.C085      IQ=IQ&N
S.C086      LL=I&(I*1-I)/2
S.C087      JQ=N&(I-2)
S.C088      DO 185 J=I,N
S.C089      JQ=JQ&N
S.C090      MM=J&(J*J-J)/2
S.C091      IF(A(LL)-A(MM)) 170,185,185
S.C092      170 X=A(LL)
S.C093      A(LL)=A(MM)
S.C094      A(MM)=X
S.C095      IF(MV-1) 175,185,175
S.C096      175 DO 180 K=1,N
S.C097      ILR=IQ&K
S.C098      IMR=JQ&K
S.C099      X=R(ILR)
S.C100      R(ILR)=R(IMR)
S.C101      180 R(IMR)=X
S.C102      185 CONTINUE
S.C103      RETURN
S.C104      END

```

SIZE OF COMMON 000000 PROGRAM 002740

END OF COMPILATION EIGEN

LEVELC 1JUL66

IBM OS/360 BASIC FORTRAN IV (E) COMPILATION

C

```
S.CC01      SUBROUTINE MATIN(ICODE,  A, ISIZE, IROW, ICOL, IS, IER)
S.CC02      DIMENSION A(1)
S.CC03      DIMENSION CARD(8)
S.CC04      1  FORMAT(7F10.0)
S.CC05      2  FORMAT(16,2I4,12)
S.CC06      IDC=7
S.CC07      IER=0
S.CC08      READ( 1,2)ICODE, IROW, ICOL, IS
S.CC09      CALL LOC(IROW, ICOL, ICNT, IROW, ICOL, IS)
S.CC10      IF(ISIZE- ICNT)6,7,7
S.CC11      6  IER=1
S.CC12      7  IF(ICNT)38,38,8
S.CC13      8  ICOLT=ICOL
S.CC14      IROCR=1
S.CC15      11 IRCDS=(ICOLT-1)/IDC&1
S.CC16      IF(IS-1)15,15,12
S.CC17      12 IRCDS=1
S.CC18      15 DO 31 K=1, IRCDS
S.CC19      READ(1,1)(CARD(I), I=1, IDC)
S.CC20      IF(IER)16,16,31
S.CC21      16 L=C
S.CC22      JS=(K-1)*IDC&ICOL-ICOLT&1
S.CC23      JE=JS&IDC-1
S.CC24      IF(IS-1)19,19,17
S.CC25      17 JF=JS
S.CC26      19 DO 30 J=JS, JE
S.CC27      IF(J-ICOL)20,20,31
S.CC28      20 CALL LOC(IROCR, J, IJ, IROW, ICOL, IS)
S.CC29      L=L&1
S.CC30      30 A(IJ)=CARD(L)
S.CC31      31 CONTINUE
S.CC32      IROCR=IROCR&1
S.CC33      IF(IROW-IROCR) 38,35,35
S.CC34      35 IF(IS-1)37,36,36
S.CC35      36 ICOLT=ICOLT-1
S.CC36      37 GO TO 11
S.CC37      38 READ(1,1) CARD(1)
S.CC38      IF(CARD(1)-9.E9)39,40,39
S.CC39      39 IER=2
S.CC40      40 RETURN
S.CC41      END
```

SIZE OF COMMON 000000 PROGRAM 001384

END OF COMPILATION MATIN

EVELC 1JUL66

IRM OS/360 BASIC FORTRAN IV (E) COMPILATION

C

```
S.0001      SUBROUTINE MXOUT (ICODE,A,N,M,MS,LINS,IPOS,ISP)
S.0002      DIMENSION A(1),B(8)
S.0003      1  FORMAT(1H1,5X,7HMATRIX,15,6X,13,5H ROWS,6X,13,8H COLUMNS,
S.0004      2  FORMAT(12X,7H COLUMN,7(3X,13,10X))
S.0005      3  FORMAT(1H )
S.0006      4  FORMAT(1H,7X,4HROW,13,7(E16.6))
S.0007      5  FORMAT(1H0,7X,4HROW,13,7(E16.6))
S.0008      J=1
S.0009      NEND=IPOS/16-1
S.0010      LEND=(LINS/ISP)-2
S.0011      IPAGE=1
S.0012      10  LSTRT=1
S.0013      20  WRITE(3,1) ICODE,N,M,MS,IPAGE
S.0014      JNT=J&NEND-1
S.0015      IPAGE=IPAGE&1
S.0016      31  IF(JNT-M)33,33,32
S.0017      32  JNT=M
S.0018      33  CONTINUE
S.0019      WRITE(3,2)(JCUR,JCUR=J,JNT)
S.0020      IF(ISP-1) 35,35,40
S.0021      35  WRITE(3,3)
S.0022      40  LTEND=LSTRT&LEND-1
S.0023      DO 80 L=LSTRT,LTEND
S.0024      DO 55 K=1,NEND
S.0025      KK=K
S.0026      JT = J&K-1
S.0027      CALL LOC(L,JT,IJNT,N,M,MS)
S.0028      B(K)=C.0
S.0029      IF(IJNT)50,50,45
S.0030      45  B(K)=A(IJNT)
S.0031      50  CONTINUE
S.0032      IF(JT-M) 55,60,60
S.0033      55  CONTINUE
S.0034      60  IF(ISP-1)65,65,70
S.0035      65  WRITE(3,4)L,(B(JW),JW=1,KK)
S.0036      GO TO 75
S.0037      70  WRITE(3,5)L,(B(JW),JW=1,KK)
S.0038      75  IF(N-L)85,85,80
S.0039      80  CONTINUE
S.0040      LSTRT=LSTRT&LEND
S.0041      GO TO 20
S.0042      85  IF(JT-M)90,95,95
S.0043      90  J=JT&1
S.0044      GO TO 10
S.0045      95  RETURN
S.0046      END
```

SIZE OF COMMON 000000 PROGRAM 001644

END OF COMPILATION MXOUT



```
S.0009      GO TO 36
S.0010      24 IRX=JX&(IX*IX-IX)/2
S.0011      GO TO 36
S.0012      30 IRX=0
S.0013      IF (IX-JX) 36,32,36
S.0014      32 IRX=IX
S.0015      36 IR=IRX
S.0016      RETURN
S.0017      END
```

```
SIZE OF COMMON 000000 PROGRAM 000752
END OF COMPILATION LOC
```

APPENDIX III

Normalization Constants

The numerical calculation of the normalization constants is very simple. The normalization constants for the HOSM wave functions are the easiest to calculate. Since there are no cross terms involved, the integrals may be evaluated by elementary means. The basic integral, involved in all of these calculations, is (17)

$$\int_0^{\infty} e^{-ax^2} x^{2n} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^{n+1} a^{n+1/2}} \sqrt{\frac{\pi}{a}}$$

For the normalization constants (there are two different values of  $\beta'$ ) of the ground state cluster model wave function, the method of App. I may be used. For the second excited state cluster model wave function, the method outlined in App. II is applicable. Here the results only are listed, without any detailed calculation.

1. Normalization constant of the cluster model wave function for the ground state:

$$N_{CM}(3/2^-) = \left\{ \begin{array}{l} 0.27025 \\ 0.29627 \end{array} \right\} \times 10^{86} \text{ cm}^{-7}$$

2. Normalization constant of the cluster model wave function for the second excited state:

$$N_{CM}(3/2^+) = 0.98167 \times 10^{100} \text{ cm}^{-5}$$

3. Normalization constants for various HOSM configurations in the ground state:

$(1s)^4(1p)^1$	$N_{SM1} = 0.27103$	} $\times 10^{86} \text{ cm}^{-7}$
$(1s)^{-1}(2s)^1$	$N_{SM2} = 0.22372$	
$(1s)^{-2}(1p)^2$	$N_{SM3} = 2.50112$	
$(1p)^{-1}(2p)^1$	$N_{SM4} = 0.10961$	
$(1s)^{-2}(2s)^2$	$N_{SM5} = 0.17328$	
$(1s)^{-1}(3s)^1$	$N_{SM6} = 0.08170$	

4. Normalization constants for various HOSM configurations in the second excited state:

$(1s)^{-1}(1p)^2$	$N_{SM1} = 0.99777 \times 10^{100} \text{ cm}^{-8}$
$(1s)^{-2}(1p)^1(2s)^1$	$N_{SM2} = 0.81157 \times 10^{100} \text{ cm}^{-8}$
$(1s)^{-2}(1p)^1(1d)^1$	$N_{SM3} = 0.45209 \times 10^{101} \text{ cm}^{-8}$
$(1s)^{-1}(2p)^1$	$N_{SM4} = 0.47028 \times 10^{100} \text{ cm}^{-8}$
$(1s)^{-3}(1p)^1(2s)^2$	$N_{SM5} = 0.66518 \times 10^{100} \text{ cm}^{-8}$

$$(1s)^{-3}(1p)^1(2s)^1(1d)^1$$

$$N_{SM6} = 0.36909 \times 10^{101} \text{ cm}^{-8}$$

$$(1s)^{-1}(1p)^{-1}(2p)^2$$

$$N_{SM7} = 0.12330 \times 10^{100} \text{ cm}^{-8}.$$

Here it should be pointed out that in the calculation of the normalization constants as well as of the other integrals some common constants have been omitted. This was pointed out in Ch. III. This has been done in all the calculations; since the same constants appear in the numerators and denominators of the final expansion coefficients, they play no role in the calculation.

APPENDIX IV

The Equivalence of the Cluster Model and the  
HOSM Wave Functions

It has been shown that if all the cluster model width parameters are equal to the HOSM width parameter for a given state (thus giving the "simple" cluster model) then the anti-symmetrized cluster model wave function for that state is identical to the antisymmetrized HOSM wave function for the corresponding state (1).

It will be shown here that the above statement is true for the ground state and the second excited state of  $\text{He}^5$ .

(a). The cluster model wave function for the ground state of  $\text{He}^5$  is given in Ch. II, Eqs. (II-3) and (II-4) are the unantisymmetrized and antisymmetrized cluster model wave functions respectively. The spatial wave function (1234;5) is given in eq.(I-1). If it is expanded in terms of the nucleon coordinates, there results

$$(1234;5) = \exp \left\{ -A(\vec{r}_1^2 + \vec{r}_2^2 + \vec{r}_3^2 + \vec{r}_4^2) - B r_5^2 - C(\vec{r}_1 \cdot \vec{r}_2 + \vec{r}_1 \cdot \vec{r}_3 + \vec{r}_1 \cdot \vec{r}_4 + \vec{r}_2 \cdot \vec{r}_3 + \vec{r}_2 \cdot \vec{r}_4 + \vec{r}_3 \cdot \vec{r}_4) - D(\vec{r}_1 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_5 + \vec{r}_3 \cdot \vec{r}_5 + \vec{r}_4 \cdot \vec{r}_5) \right\} \left[ \frac{1}{2}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_5 \right] Y_1^1(\Omega_{R_1})$$

where

$$A = \frac{2}{8} \mu_1, \quad B = \frac{1}{10} \beta' + \frac{\mu_1}{10}, \quad C = \frac{2}{4} \alpha_1 + \frac{\beta'}{20} + \frac{1}{5} \mu_1, \quad D = \frac{1}{5} (\mu_1 - \beta').$$

If the cluster model width parameters  $\alpha_1, \beta'$  are made equal

to the HOSM width parameter  $\mu_1$ , then

$$A = \frac{1}{2} \mu_1, \quad B = \frac{1}{2} \mu_1, \quad C = D = 0.$$

The cluster model wave function then becomes

$$\phi_{CM} = N_{CM} \exp(-\frac{1}{2} \mu_1 \sum_{i=1}^5 r_i^2) \left[ \frac{1}{4} (\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_5 \right] Y_1^1(\Omega_{R_1}) \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5.$$

If the antisymmetrization operator  $\mathcal{A}$  is applied as in Ch. 2 there results

$$\mathcal{A} \phi_{CM} = N_{CM} \exp(-\frac{1}{2} \mu_1 \sum_{i=1}^5 r_i^2) \mathcal{A} \left\{ \left[ \frac{1}{4} (\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_5 \right] Y_1^1(\Omega_{R_1}) \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \right\}$$

This simplification occurs because  $\exp(-\frac{1}{2} \mu_1 \sum_{i=1}^5 r_i^2)$  is a totally symmetric function of the five coordinates and therefore can be ignored while carrying out the antisymmetrization. Thus, there remains only (1)

$$\begin{aligned} & \mathcal{A} \left\{ R_1 Y_1^1(\Omega_{R_1}) \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \right\} \\ &= \mathcal{A} \left\{ R_1 \sin \theta_{R_1} (\cos \phi_{R_1} + i \sin \phi_{R_1}) \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \right\} \\ &= \mathcal{A} \left\{ (x + iy) \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \right\} \\ &= \mathcal{A} \left\{ \frac{1}{4} \left[ (x_1 + iy_1) + (x_2 + iy_2) + (x_3 + iy_3) + (x_4 + iy_4) - 4(x_5 + iy_5) \right] \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \right\} \\ &= \mathcal{A} \left\{ \sum_{j,k,\dots,l=1}^5 \left[ \text{const.} \times (x_j + iy_j)^{n_j} (x_k + iy_k)^{n_k} \dots (x_l + iy_l)^{n_l} \right] \right. \\ & \qquad \qquad \qquad \left. \times \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \right\} \end{aligned}$$

where  $n_j + n_k + \dots + n_l = 1$ . Therefore

$$\mathcal{A} \phi_{CM} = \mathcal{A} N_{CM} \left\{ \exp(-\frac{1}{2} \mu_1 \sum_{i=1}^5 r_i^2) (x_j + iy_j) \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \right\}$$

$$= A N_{CM} \left\{ \exp(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2) \vec{r}_5 Y_1^1(\Omega_5) \alpha_1 \beta_2 \alpha_3 \beta_4 \alpha_5 \right\}.$$

When this wave function is normalized, the constants are equal

$N_{CM} = N_{SML}$ , so that

$$A \phi_{CM}(3/2-; \alpha_1 = \beta' = \mu_1) = A \phi_{SML}(3/2-).$$

If a scalar product of the  $\phi_{SML}$  is formed with  $A \phi_{CM}(3/2-;$

$\alpha_1 = \beta' = \mu_1)$ , then  $a_1=1$  and  $a_2=a_3=a_4=a_5=a_6=0$ . This check has been carried out by computation and is shown in Fig. 4.

(ii). This sort of equivalence can also be shown for the second excited state; the cluster model spatial wave function for this state is

$$(123;45) = \exp \left\{ -A(r_1^2 + r_2^2 + r_3^2) - B(r_4^2 + r_5^2) - C(\vec{r}_1 \cdot \vec{r}_2 + \vec{r}_1 \cdot \vec{r}_3 + \vec{r}_2 \cdot \vec{r}_3) + D(\vec{r}_1 \cdot \vec{r}_4 + \vec{r}_1 \cdot \vec{r}_5 + \vec{r}_2 \cdot \vec{r}_4 + \vec{r}_2 \cdot \vec{r}_5 + \vec{r}_3 \cdot \vec{r}_4 + \vec{r}_3 \cdot \vec{r}_5) - E \vec{r}_4 \cdot \vec{r}_5 \right\} R^2 Y_0^0(\Omega_R)$$

where

$$A = \frac{\alpha}{3} + \frac{\beta}{15} + \frac{\mu_1}{10}, \quad B = \frac{1}{2}\bar{\alpha} + \frac{3}{20}\beta + \frac{\mu_1}{10}, \quad C = \frac{1}{3}\alpha + \frac{2}{15}\beta + \frac{\mu_1}{5}, \quad D = \frac{1}{5}(\mu_1 - \beta),$$

$$E = -\frac{1}{2}\bar{\alpha} + \frac{3}{10}\beta + \frac{\mu_1}{5}.$$

If  $\alpha = \bar{\alpha} = \beta = \mu_1$ , then

$$(123;45) = \exp(-\frac{1}{2}\mu_1 \sum_{i=1}^5 r_i^2) R^2 Y_0^0(\Omega_R).$$

Using the same procedure as for the ground state wave function,

there results

$$A \phi_{CM}(3/2+; \alpha = \bar{\alpha} = \beta = \mu_1) = A \phi_{SML}(3/2+).$$

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

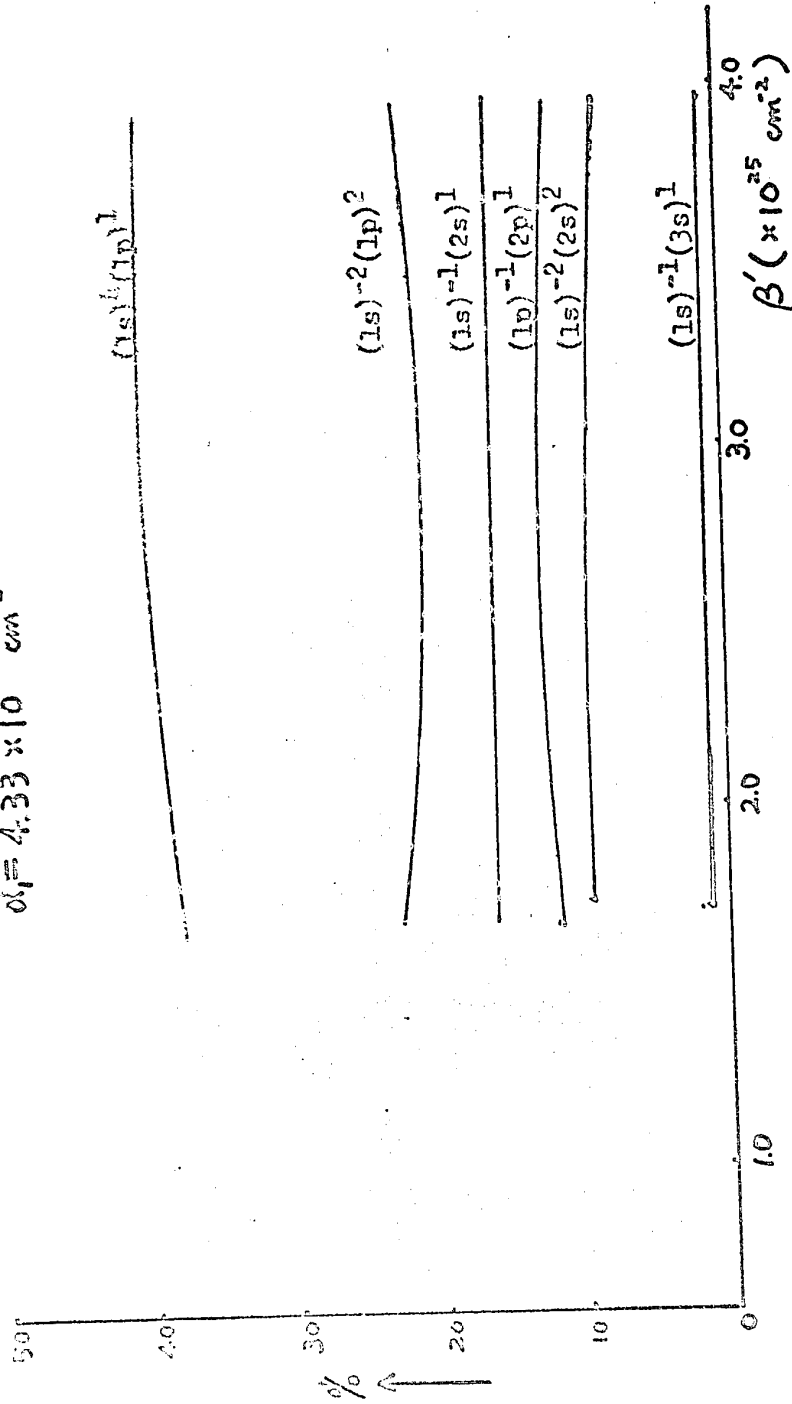


Fig. 2. The intensities of the different configurations found in the ground state cluster model wave function with constant  $\alpha_1$ , as functions of  $\beta'$ .

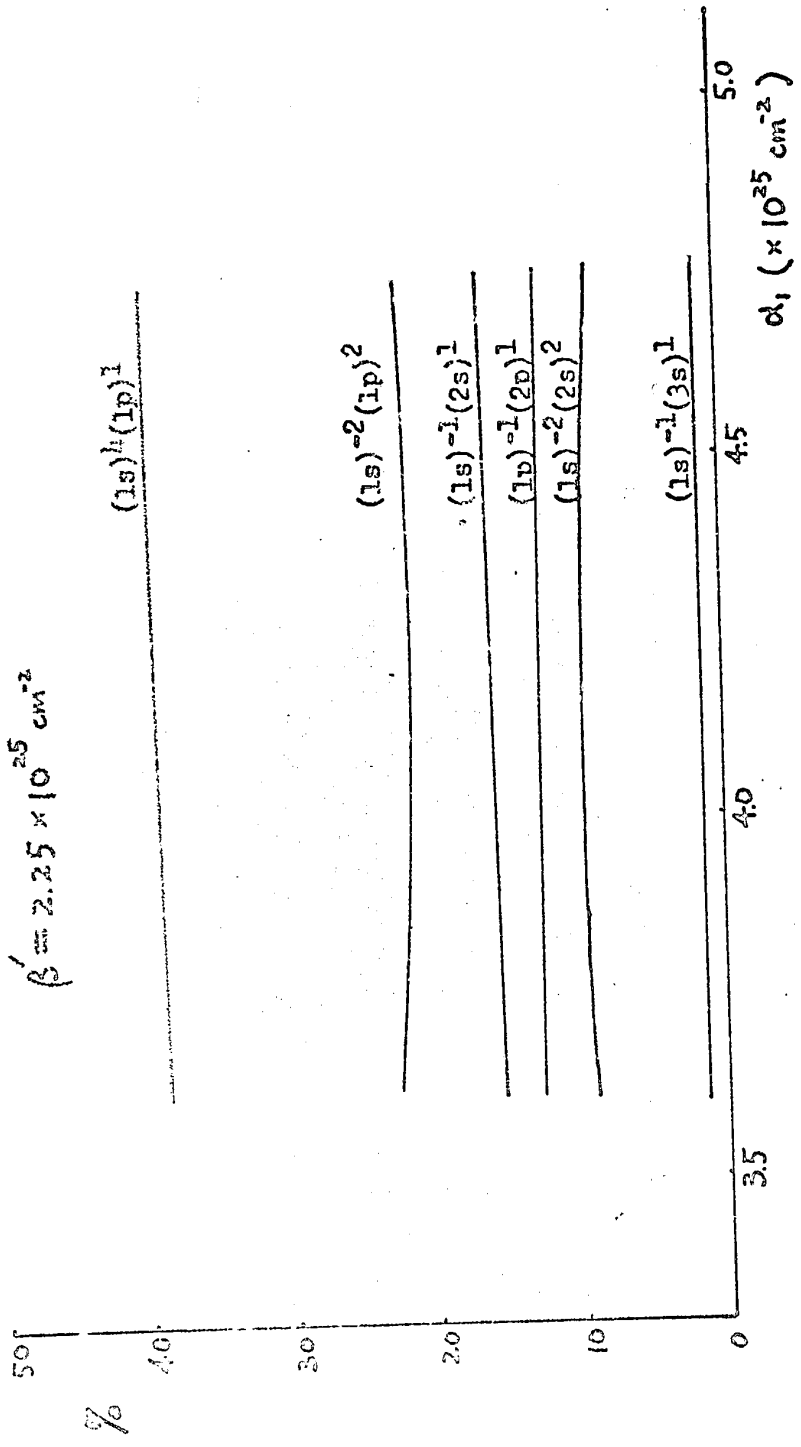


Fig. 3. The intensities of the different configurations found in the ground state cluster model wave function with constant  $\beta'$ , as functions of  $\alpha_1$ .

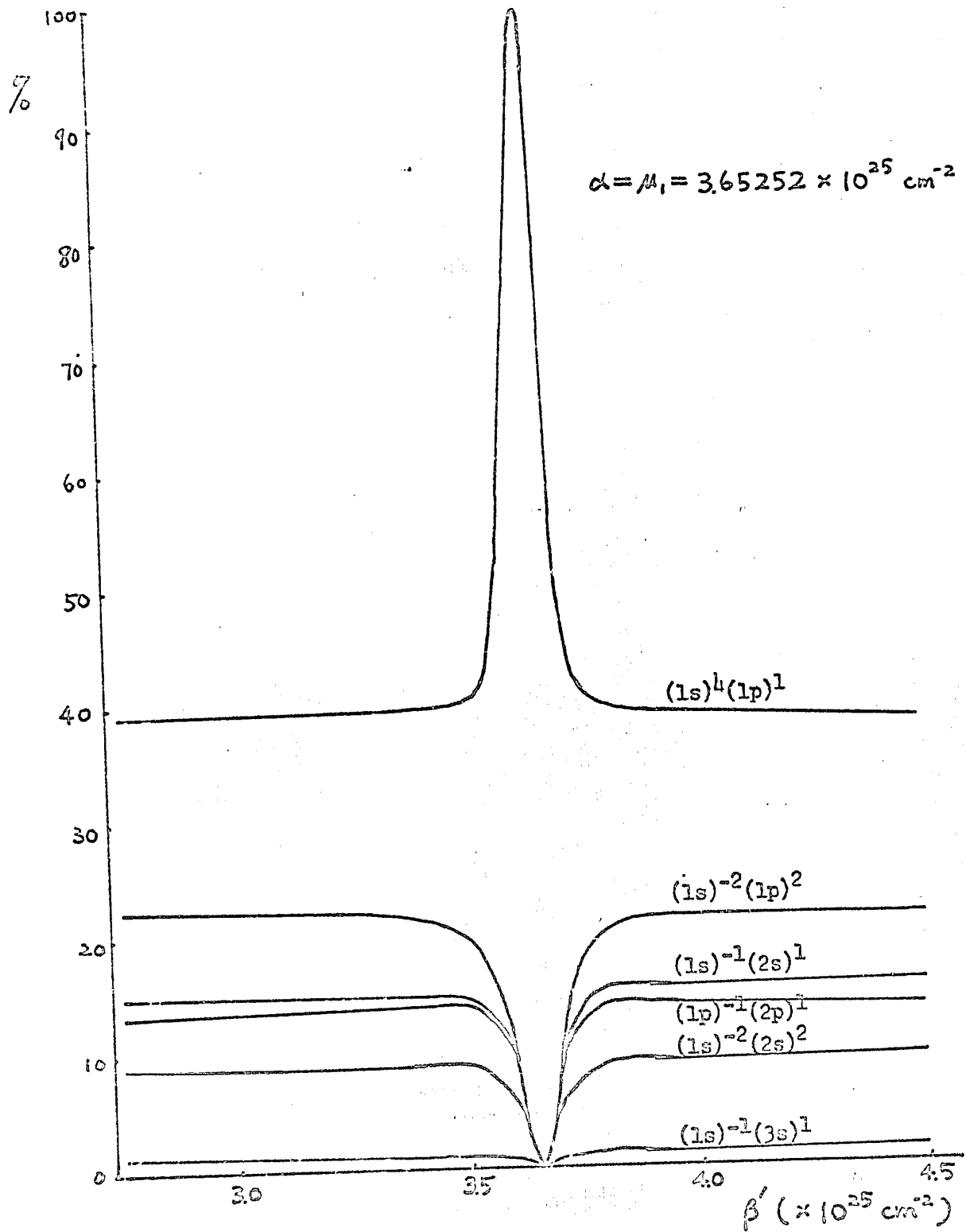


Fig. 4. The intensities of the different configurations found in the ground state cluster model wave function with constant  $\alpha = \mu_1$  as functions of  $\beta'$ .

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