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Antisymmetrization of "Cluster Model" Wave Functions
and
Expansion in Single Particle "Shell Model" Wave Functions
by

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A B S T R A C T.

A method is described whereby oscillator "Cluster Model" wave functions may be antisymmetrized and expressed as a superposition of "Shell Model" wave functions. Moreover, some ideas are presented concerning the antisymmetrization of wave functions in general. For the Cluster Model calculations, they are useful when passing from the oscillator wave functions to more general cluster wave functions.

INTRODUCTION

This note deals with possible ways of antisymmetrization of oscillator "cluster model" wave functions ^{1) 2) 3)} and expressing them as a superposition of single particle wave functions ^{*)}.

The choice of a convenient notation simplifies greatly the calculations. This is why in Part I the notation which is used is explained in some details, and properties of this notation are derived.

In Part II we discuss a method by which one can obtain antisymmetrized cluster model wave functions quickly for nuclear states in which there are no nucleons outside of the $1p$ shell.

With the method which is described in Part III, it is possible to construct any antisymmetric oscillator "cluster model" wave functions. The antisymmetrization is carried out mainly in two steps, i.e. first we obtain the antisymmetric wave functions for the clusters and second we extend the antisymmetrization over all the particles. For the first step, the method of Part II is usually very useful.

Finally, in Part IV, we put down some ideas in which any wave function can be antisymmetrized and some preliminary conclusions are derived. One needs such a method if one wants to generalize the cluster model wave functions, i.e. when one gets away from the oscillator model wave functions.

*) The reason why it is very useful to expand the cluster model wave functions in single particle wave functions, is **that** one can see directly their orthogonality and obtain their normalization factors very easily.

(iii) In writing down a Slater determinant, as in (1), the order of the elements is irrelevant, because exchange of two diagonal elements in a determinant means exchange of two rows and two columns simultaneously. For example :

$$u_1^1(1)u_2^2(2)u_3^4(3) = u_1^1(1)u_3^4(3)u_2^2(2)$$

This enables us to assume that we can always write the "representative" diagonal in such a way that the particles are arranged in increasing order and therefore we can drop the corresponding index. It is also convenient to extend the notation of § ii to any positive integral index, by assuming that all indices of the form $4n+j$ belong to the same spin and i -spin state as j .

Now with this notation it is easy to verify that :

$$\dots u^i \dots v^j \dots = - \dots v^j \dots u^i \dots \quad (3)$$

and that :

$$\dots u^i \dots v^j \dots \quad \text{and} \quad \dots v^i \dots u^j \dots$$

are quite different functions unless $i \equiv j \pmod{4}$ in which case :

$$\dots u^i \dots v^j \dots = - \dots v^i \dots u^j \dots \quad i \equiv j \pmod{4} \quad (4)$$

(iv) If we have a product of two (or more) Slater determinants with no common particles, the completely anti-symmetric expression is one Slater determinant which has, as principal diagonal, the "sum" of the diagonals of the factor

determinants. Thus we have, for example :

$$\begin{aligned} A \{ (u^\alpha(1) u^\beta(2) \dots u^\tau(n) \cdot (v^\mu(n+1) \dots v^\sigma(N))) \} = \\ = u^\alpha(1) u^\beta(2) \dots u^\tau(n) v^\mu(n+1) \dots v^\sigma(N) \end{aligned} \quad (5)$$

The l.h.s. of (5) is the Lagrange expansion of the determinant of the r.h.s. with respect to the first n columns. A in the l.h.s. stands for the antisymmetrization operator.

(v) Suppose now we have a Slater determinant $D(n)$ for n particles. We can write the columns in four groups. The first group corresponds to states of protons with spin "up", the second to protons with spin "down" and third and fourth to neutrons with spin "up" and "down" respectively. Let us say that n_1, n_2, n_3, n_4 are the numbers of columns in these groups. We have

$$n_1 + n_2 + n_3 + n_4 = n$$

So we may always write :

$$D(n) = \begin{vmatrix} u_1^1(1) u_2^1(1) \dots u_{n_1}^1(1) & v_1^2(1) \dots v_{n_2}^2(1) & w_1^3(1) \dots w_{n_3}^3(1) & t_1^4(1) \dots t_{n_4}^4(1) \\ u_1^1(2) u_2^1(2) \dots u_{n_1}^1(2) & v_1^2(2) \dots v_{n_2}^2(2) & w_1^3(2) \dots w_{n_3}^3(2) & t_1^4(2) \dots t_{n_4}^4(2) \\ u_1^1(3) u_2^1(3) \dots u_{n_1}^1(3) & v_1^2(3) \dots v_{n_2}^2(3) & w_1^3(3) \dots w_{n_3}^3(3) & t_1^4(3) \dots t_{n_4}^4(3) \\ \dots & \dots & \dots & \dots \\ u_1^1(n) u_2^1(n) \dots u_{n_1}^1(n) & v_1^2(n) \dots v_{n_2}^2(n) & w_1^3(n) \dots w_{n_3}^3(n) & t_1^4(n) \dots t_{n_4}^4(n) \end{vmatrix} \quad (6)$$

Taking into account § iv we can write $D(n)$ as :

$$D(n) = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n_1} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n_2} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_{n_3} \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_{n_4} \end{pmatrix} \quad (7)$$

Here we do not care about antisymmetrization in spin and i-spin space, as each column corresponds to a definite spin and i-spin wave function. Each of the above columns is the principal diagonal of the partial determinant in which the $D(n)$ can be expanded (Lagrange method). The complete determinant is obtained by combining the four columns. This shows that we can take one distribution of the n particles on the four spin and i-spin states and carry out the antisymmetrization only over the spatial co-ordinates in constructing the four partial determinants. The totally antisymmetric function is then obtained by combining these four determinants, and in our notation, it is enough to write expression (7).

From the construction of (7) it is easy to see that by interchanging two states of the same column, the whole expression changes sign. If we interchange two states between two different columns, we obtain an expression which is a quite different wave function.

(vi) In this paragraph we shall show how, in our notation, an operator symmetric in n particles acts on a Slater determinant. We start with the identity

$$\sum_{i < j < k \dots < r}^n \begin{vmatrix} a_{i1} & a_{i2} & \dots & a_{in} \\ \vdots & \vdots & \ddots & \vdots \\ a'_{i1} & a'_{i2} & \dots & a'_{in} \\ \vdots & \vdots & \ddots & \vdots \\ a'_{j1} & a'_{j2} & \dots & a'_{jn} \\ \vdots & \vdots & \ddots & \vdots \\ a'_{k1} & a'_{k2} & \dots & a'_{kn} \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ a'_{r1} & a'_{r2} & \dots & a'_{rn} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{vmatrix} = \sum_{i < j < k \dots < r}^n \begin{vmatrix} a_{i1} \dots a'_{i1} \dots a'_{ij} \dots a'_{ik} \dots a'_{ir} \dots a_{in} \\ a_{21} \dots a'_{2i} \dots a'_{2j} \dots a'_{2k} \dots a'_{2r} \dots a_{2n} \\ \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \\ \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \\ a_{n1} \dots a'_{ni} \dots a'_{nj} \dots a'_{nk} \dots a'_{nr} \dots a_{nn} \end{vmatrix} \quad (8)$$

which is easy to prove by expanding each determinant at the l.h.s. along the $i, j, k, \dots r^{\text{th}}$ rows and those on the r.h.s. along the $i, j, k, \dots r^{\text{th}}$ columns. Without loss of generality we can take a two particles symmetric operator to illustrate its effect in the adopted notation.

We have :

$$\begin{aligned} \sum_{i < j}^n O_{ij} (u_1 u_2 \dots u_n) &= \sum_{i < j}^n O_{ij} \begin{vmatrix} u_1(1) & u_2(1) & \dots & u_n(1) \\ u_1(2) & u_2(2) & \dots & u_n(2) \\ \cdot & \cdot & \cdot & \cdot \\ u_1(n) & u_2(n) & \dots & u_n(n) \end{vmatrix} = \\ &= \sum_{i < j}^n \begin{vmatrix} u_1(1) & u_2(1) & \dots & u_n(1) \\ \cdot & \cdot & \cdot & \cdot \\ u'_1(i) & u'_2(i) & \dots & u'_n(i) \\ \cdot & \cdot & \cdot & \cdot \\ u'_1(j) & u'_2(j) & \dots & u'_n(j) \\ \cdot & \cdot & \cdot & \cdot \\ u_1(n) & u_2(n) & \dots & u_n(n) \end{vmatrix} = \sum_{i < j}^n \begin{vmatrix} u_1(1) \dots u'_i(1) \dots u'_j(1) \dots u_n(1) \\ u_1(2) \dots u'_i(2) \dots u'_j(2) \dots u_n(2) \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ u_1(n) \dots u'_i(n) \dots u'_j(n) \dots u_n(n) \end{vmatrix} = \\ &= \sum_{i < j}^n (u_1 u_2 \dots u'_i \dots u'_j \dots u_n) \end{aligned} \quad (9)$$

[with the convention $O_{ij} u_{\alpha}(i) u_{\beta}(j) = u'_{\alpha}(i) u'_{\beta}(j)$]

At this point we have to note that when an operator acts on the spin or i-spin states, this sometimes corresponds to transferring a state from one column to another in expression (7). We have then to take into account the change in sign, if the displacement is along an odd number of places.

(vii) Another application of the identity (8) is the following: Suppose we want to antisymmetrize the expression

$$K = \{u_1(1)u_2(2)\dots u_n(n)\} \cdot v(k)$$

where the expression in the bracket is a Slater determinant represented by its principal diagonal and k is one of the particles $1, \dots, n$. Then

$$AK = \{u_1(1)u_2(2)\dots u_n(n)\} \sum_{k=1}^n v(k) = \sum_{k=1}^n u_1(1)u_2(2)\dots \overline{u_k(k)} v(k) \dots u_n(n)$$

Similarly if

$$K = \{u_1(1)\dots u_n(n)\} \cdot v(k)w(\ell) \quad \text{with } k \text{ and } \ell \text{ in } 1, 2, \dots, n$$

then

$$AK = \sum_{k < \ell}^n u(1)\dots \overline{u_k(k)} v(k) \dots \overline{u_\ell(\ell)} w(\ell) \dots u_n(n)$$

where A is the antisymmetrization operator.

(ix) Suppose we have n elements

$$a_1, a_2, a_3, \dots, a_n$$

which are arranged in a definite order denoted by their indices. We call any combination of these elements taken in groups of ℓ , even or odd, according to whether the sum of the indices of the elements in the combination is even or odd.

For example, the combinations of nC_3 , $a_1a_3a_5$ or $a_2a_3a_6$ are odd, while the combinations $a_1a_3a_5$ or $a_7a_9a_{10}$ are even. The sum of the indices in a given combination is denoted by $[{}^nC_\ell]$.

With this notation it is easy to write down an expression for the expansion of a determinant according to the Lagrange method.

$$\begin{vmatrix} a_{11} & a_{12} & \dots & a_{1\ell} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2\ell} & \dots & a_{2n} \\ \cdot & \cdot & \dots & \cdot & \dots & \cdot \\ a_{n1} & a_{n2} & \dots & a_{n\ell} & \dots & a_{nn} \end{vmatrix} = (-1)^{\frac{\ell(\ell+1)}{2}} \sum_{{}^nC_\ell} (-1)^{[{}^nC_\ell]} \begin{vmatrix} a_{j_1} & a_{j_2} & \dots & a_{j_\ell} \\ a_{i_1} & a_{i_2} & \dots & a_{i_\ell} \\ \cdot & \cdot & \dots & \cdot \\ a_{k_1} & a_{k_2} & \dots & a_{k_\ell} \end{vmatrix} \times \begin{vmatrix} a_{m_{\ell+1}} & \dots & a_{mn} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ a_{s_{\ell+1}} & \dots & a_{sn} \end{vmatrix} \quad (9a)$$

with $[{}^nC_\ell] = j + i + \dots + k$

where $\sum_{{}^nC_\ell}$ means sum over all combinations ${}^nC_\ell$.

II Antisymmetrization of some expressions involving single particle wave functions:

In this part we deal with the antisymmetrization of expressions of the form :

$$f = (a_{11}u_1^1 + a_{12}u_1^2 + \dots + a_{1n}u_1^n)^{m_1} (a_{21}u_2^1 + a_{22}u_2^2 + \dots + a_{2n}u_2^n)^{m_2} \dots \dots \dots (a_{e1}u^1 + \dots + a_{en}u^n)^{m_e} \quad (10)$$

with m_j 's integer numbers and

$$m_1 + m_2 + m_3 + \dots + m_e = n \quad (11)$$

where n is the number of particles.

The u_i^ℓ 's are single particle functions and $a_{i\ell}$ are numerical coefficients. The superscripts in u_i^ℓ number the particles and at the same time denote the spin and i-spin. In a given bracket of (10), the u 's all have the same spatial part.

We can express many wave functions for the Cluster Model in the form (10). If we use the harmonic oscillator functions, the u_i^ℓ 's are Hermite Polynomials. The wave functions for all nuclei up to O^{16} can be directly represented by expressions similar to (10), but for heavier nuclei there are difficulties in putting the wave functions in this form ^{*)}. In part III, a

^{*)} Strictly speaking, in form (10) we can put the Cluster wave functions for nuclear states, in which there are no nucleons outside of the lp shell.

more general method for antisymmetrization of the Cluster Model wave functions will be given. However, we think it is useful to explain here a method of antisymmetrization of (10) which can be easily extended to the case where the u 's are any kind of single particle functions.

The antisymmetrization of (10) can be done by expanding this expression and considering each term of the expansion as the principal diagonal of a Slater determinant for n particles.

In this way, many terms of the expansion will vanish, while others will be identical. However, the expansion of (10) is not practicable because the number of terms increases very rapidly with n . Our task is to give a method by which we can obtain directly the final result.

Because of (11) we have to consider only those terms of the expansion which are linear in the u 's, as every term has to contain functions for all n particles. We suppose that we write these terms as in (7). Let n_1, n_2, n_3, n_4 be the numbers of particles in the first, second, third and fourth columns. We have :

$$n_1 + n_2 + n_3 + n_4 = n$$

Consider one term of the expansion :

$$m_1! m_2! \dots m_p! a_{11} a_{25} \dots a_{\tau, 4\lambda+1} \dots \begin{pmatrix} u_1^1 \\ u_2^1 \\ \vdots \\ u_{4\lambda+1}^1 \\ \vdots \end{pmatrix} \begin{pmatrix} u_1^2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{pmatrix} \begin{pmatrix} u_1^3 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{pmatrix} \begin{pmatrix} u_1^4 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{pmatrix} \quad (12)$$

The functions in each column must have been taken from different brackets of (10), otherwise (12) is identically zero. Next consider all other terms in the expansion which differ from (12) in the first column only. Some of these arise from (12) by permutation of the superscripts in the first column, and hence are the same apart from their numerical coefficients. Collecting them together it is easy to see that they form the expansion of the determinant :

$$Q_1^{\ell}(\begin{smallmatrix} n_1 \\ p \end{smallmatrix}) = \begin{vmatrix} a_{11}a_{15}\cdots a_{1,4r+1} \\ a_{21}a_{25}\cdots a_{2,4r+1} \\ - & - & - & - \\ a_{\tau 1}a_{\tau 5}\cdots a_{\tau,4r+1} \end{vmatrix} \quad (13)$$

where $r = n_1 - 1$.

The indices on the u 's in (12) are the same as the subscripts on the principal diagonal of (13). If we change the order of the elements in (12) we have a corresponding change in the order of the rows in (13) with the result that there is no change in sign in the final expression. Another choice of n_1 u 's from the e brackets will give another coefficient $Q_1^j(\begin{smallmatrix} n_1 \\ e \end{smallmatrix})$. Similarly we can construct the coefficients $Q_2^k(\begin{smallmatrix} n_2 \\ e \end{smallmatrix})$, $Q_3^h(\begin{smallmatrix} n_3 \\ p \end{smallmatrix})$ and $Q_4^g(\begin{smallmatrix} n_4 \\ p \end{smallmatrix})$ for the other columns. The coefficients of really distinct terms of Af are of the form :

$$Q_1^j(\begin{smallmatrix} n_1 \\ p \end{smallmatrix}) Q_2^k(\begin{smallmatrix} n_2 \\ e \end{smallmatrix}) Q_3^{\ell}(\begin{smallmatrix} n_3 \\ e \end{smallmatrix}) Q_4^m(\begin{smallmatrix} n_4 \\ e \end{smallmatrix}) \quad (14)$$

The functional part of any term is obtained by using the subscripts of the elements in the principal diagonals of the Q 's as the indices of the u 's in the corresponding columns.

The number of terms which one obtains is in principle $\rho_{C_{n1}} \cdot \rho_{C_{n2}} \cdot \rho_{C_{n3}} \cdot \rho_{C_{n4}}$. In practice, however, this number is reduced, because usually there exist some relations among the a_{ij} 's.

From the way (13) is constructed, one derives that :

(i) We must have :

$$n_i \leq \rho \quad (i = 1, 2, 3, 4) \quad (15)$$

If for one n_i we have n_i then $Af = 0$.

(ii) If all the coefficients a_{ij} in (10) are equal (or proportional), then $Af = 0$

(iii) If the coefficients a_{ij} , corresponding to the k^{th} column in (12) for at least $\rho - n + 2$ brackets are proportional, then $Af = 0$, because in every determinant (13), for the k^{th} column, there will be at least two rows with proportional elements. In practice we have many brackets with corresponding coefficients equal. This reduces the number of Q 's and therefore the number of terms in the final expression.

(iv) Suppose that the ρ brackets can be divided with respect to the i^{th} column, in ν_i groups, so that in

the
every group corresponding to the i^{th} column, coefficients of the different brackets are equal. Then we can put instead of (15)

$$n_i \leq v_i < p \quad (15a)$$

and the number of the terms is reduced to

$${}^i C_{n_1} \quad {}^i C_{n_2} \quad {}^3 C_{n_3} \quad {}^4 C_{n_4}$$

(v) In the expression (10), it is possible that two brackets contain the same functions u 's but with different coefficients a_{ij} , i.e. :

$$u_l^i = u_h^i$$

but

$$a_{li} \neq a_{hi}$$

In this case, terms containing states from both brackets l and h and referred to the same column vanish, not from the coefficients Q but from their adjusted Slater determinants, which will contain two particles in the same state. This also will reduce the number of terms in the final expression.

Note:

If we suppose, with harmonic oscillator wave functions that s shell is filled, then the coefficients (13) become

$$Q_1 \binom{n_1-1}{p} = (-)^{n_1-1} \begin{vmatrix} 1 & 1 & \dots & 1 \\ a_{11} & a_{15} & \dots & a_{1,4} & +1 \\ - & - & - & - & - \\ a_{11} & a_{22} & \dots & a_{,4} & +1 \end{vmatrix} \quad (13a)$$

with $r_1 = n_1 - 1$. We obtain similar expressions for $Q_2^3 \binom{n_2-1}{p}$, $Q_3^k \binom{n_3-1}{p}$, $Q_4^m \binom{n_4-1}{p}$. This is because we have n_i elements in the i^{th} column of (12) in which one is always supposed to be the 1s state and so one less is chosen from the $u_{i\ell}$'s. So we get as corresponding coefficient, the sum of n_i determinants which is exactly the expansion of (13a).

Examples:

We illustrate below the method with some examples. They are applications of the Cluster Model wave functions to light nuclei. We use harmonic oscillator wave functions.

For convenience, we put for the P shell wave functions:

$$\begin{aligned} P_{10} &\propto a = z \\ P_{11} &\propto b = x + iy \\ P_{1-1} &\propto c = x - iy \end{aligned} \quad (16)$$

a) Ground state of Be^8

We consider that the ground state of Be^8 is formed by two α -particles in a 3s relative oscillation. So before antisymmetrization, we can write :

$$\psi^{\text{Be}^8} = f_{1s}(\alpha_1) f_{1s}(\alpha_2) X_{3s}(\alpha_1 - \alpha_2) \quad (17)$$

The polynomial ^{*)} part of (17) with which we shall be concerned is :

$$X_{3s}(R_{12}) \propto R_{12}^4 - \frac{5}{\alpha} R_{12}^2 + \frac{15}{4\alpha^2} \quad \text{**)} \quad (17a)$$

^{*)} The exponential part of (17) is symmetric in all the particles.

^{**)} The polynomial parts of $f_{1s}(\alpha_1)$ and $f_{1s}(\alpha_2)$ are both constants.

with

$$\underline{R}_{12} = \frac{r_1+r_2+r_3+r_4}{4} - \frac{r_5+r_6+r_7+r_8}{4}$$

The second and the third terms of (17a) after anti-symmetrization vanish as they correspond to states with six and eight particles in the 1s state respectively.

It remains therefore the antisymmetrization of the term :

$$R_{12}^4 = (a_{12}^2 + b_{12}c_{12})^2 = a_{12}^4 + 2a_{12}^2 b_{12}c_{12} + b_{12}^2 c_{12}^2 \quad (17b)$$

where

$$a_{12} = \frac{a_1+a_2+a_3+a_4}{4} - \frac{a_5+a_6+a_7+a_8}{4}$$

$$b_{12} = \frac{b_1+b_2+b_3+b_4}{4} - \frac{b_5+b_6+b_7+b_8}{4}$$

$$c_{12} = \frac{c_1+c_2+c_3+c_4}{4} - \frac{c_5+c_6+c_7+c_8}{4}$$

We have to antisymmetrize separately a_{12}^4 , $a_{12}^2 \cdot b_{12} \cdot c_{12}$ and $b_{12}^2 \cdot c_{12}^2$.

$$1) \quad a_{12}^4 = \frac{1}{4} \{ (a_1+a_2+a_3+a_4) - (a_5+a_6+a_7+a_8) \}^4$$

Here $p=1$ and $n_1=n_2=n_3=n_4=2$. Therefore :

$$Q_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix} = Q_2 \begin{pmatrix} 1 \\ 1 \end{pmatrix} = Q_3 \begin{pmatrix} 1 \\ 1 \end{pmatrix} = Q_4 \begin{pmatrix} 1 \\ 1 \end{pmatrix} = (-)^1 \begin{vmatrix} 1 & 1 \\ 1 & -1 \end{vmatrix} = 2$$

So

$$A a_{12}^4 = 4! \frac{2^4}{4^4} (\overset{s}{a})(\overset{s}{a})(\overset{s}{a})(\overset{s}{a}) = \frac{4!}{16} (\overset{s}{a})(\overset{s}{a})(\overset{s}{a})(\overset{s}{a}) \quad *)$$

$$\begin{aligned} 2/ \quad a_{12}^2 b_{12} c_{12} &= \frac{1}{4^4} \left[(a_1 + \dots + a_4) - (a_5 + \dots + a_8) \right]^2 \\ &\quad \times \left[(b_1 + \dots + b_4) - (b_5 + \dots + b_8) \right] \times \\ &\quad \times \left[(c_1 + \dots + c_4) - (c_5 + \dots + c_8) \right] \end{aligned}$$

Again $Q_1^i = Q_2^i = Q_3^i = Q_4^i = 2$. Therefore :

$$A a_{12}^2 b_{12} c_{12} = \frac{2!}{4^4} 2^4 \overline{(\overset{s}{a})(\overset{s}{a})(\overset{s}{b})(\overset{s}{c})} = \frac{2!}{16} \overline{(\overset{s}{a})(\overset{s}{a})(\overset{s}{b})(\overset{s}{c})}$$

where the bar over the expression means that we have to take the sum of all the different permutations of the columns.

$$3/ \quad b_{12}^2 c_{12}^2 = \frac{1}{4^4} \left[(b_1 + \dots + b_4) - (b_5 + \dots + b_8) \right] \left[(c_1 + \dots + c_4) - (c_5 + \dots + c_8) \right]^2$$

We find similarly :

$$A b_{12}^2 c_{12}^2 = \frac{2! 2!}{4} 2^4 \overline{(\overset{s}{b})(\overset{s}{b})(\overset{s}{c})(\overset{s}{c})}$$

The final expression for the antisymmetrized wave function of

*) **s** in the bracket denotes the 1s state.

Be^8 in the ground state is :

$$\Psi \propto 6(\frac{s}{a})(\frac{s}{a})(\frac{s}{a})(\frac{s}{a}) + \overline{(\frac{s}{a})(\frac{s}{a})(\frac{s}{b})(\frac{s}{c})} + \overline{(\frac{s}{b})(\frac{s}{b})(\frac{s}{c})(\frac{s}{c})}$$

It is the sum of 19 terms. If we write a, b, c, again for the normalized wave functions P_{10}, P_{11}, P_{1-1} , we have :

$$\Psi_{\text{normalized}} = \frac{1}{\sqrt{45}} \{ 3 (\frac{s}{a})(\frac{s}{a})(\frac{s}{a})(\frac{s}{a}) + \overline{(\frac{s}{a})(\frac{s}{a})(\frac{s}{b})(\frac{s}{b})} + 2 \overline{(\frac{s}{b})(\frac{s}{b})(\frac{s}{c})(\frac{s}{c})} \}$$

b) 2^+ State of C^{12} :

We take $J = 2, J_z = 2$.

This state in the Cluster Model can be described as Be^8 oscillating against an α -particle. There are many expressions for this state as, for example :

$$F(\text{Be}^8)_{3S} \cdot f_{1S}(\alpha) \cdot X_{(\text{Be}^8 \leftrightarrow \alpha)_{2D}}$$

or
$$F(\text{Be}^8)_{2D} \cdot f_{1S}(\alpha) \cdot X_{(\text{Be}^8 \leftrightarrow \alpha)_{3S}}$$

$$F(\text{Be}^8)_{2D} \cdot f_{1S}(\alpha) \cdot X_{(\text{Be}^8 \leftrightarrow \alpha)_{2D}}$$

etc.

but after antisymmetrization, all lead to the same final expression.

We take the first one. The polynomial parts are :

$$F(\text{Be}^8)_{3S} \propto 15 - 20\alpha r'^2 + 4\alpha^2 r'^4 = 15 - 20\alpha(a' + b'c') + 4\alpha^2(a'^2 + b'c')^2$$

$$f_{1S}(\alpha) \propto 1$$

$$(\text{Be}^8 \leftrightarrow \alpha)_{2D_2} \propto b''^3 c'' + a''^2 b''^2$$

where

$$\begin{aligned} b' &= \frac{b_1 + \dots + b_4}{4} - \frac{b_5 + \dots + b_8}{4} \\ c' &= \frac{c_1 + \dots + c_4}{4} - \frac{c_5 + \dots + c_8}{4} \\ a' &= \frac{a_1 + \dots + a_4}{4} - \frac{a_5 + \dots + a_8}{4} \end{aligned}$$

and

$$\begin{aligned} b'' &= \frac{b_1 + \dots + b_8}{8} - \frac{b_9 + \dots + b_{12}}{4} \\ c'' &= \frac{c_1 + \dots + c_8}{8} - \frac{c_9 + \dots + c_{12}}{4} \\ a'' &= \frac{a_1 + \dots + a_8}{8} - \frac{a_9 + \dots + a_{12}}{4} \end{aligned}$$

From the F_{3s} we keep only the highest term as the others lead to expressions which vanish after antisymmetrization, because there will be more than 4 particles in the 1s state.

We have to antisymmetrize the expression :

$$\begin{aligned} (a'^2 + b'c')^2 (b''^3 c'' + a''^2 b''^2) &= (a'^4)(b''^3 c'') + 2(a'^2 b'c')(b''^3 c'') + \\ &+ 2(a'^2 b'c')(a''^2 b''^2) + (b'^2 c'^2)(a''^2 b''^2) + \\ &+ (a'^4)(a''^2 b''^2) + (b'^2 c'^2)(b''^3 c'') \end{aligned}$$

The last two terms give zero after antisymmetrization because in the last one there are 5 states b and in the other 6 states a .

We have $n_1=n_2=n_3=n_4=3$ and the Q 's are 3×3 determinants. It is easy to see that they are all equal to :

$$(-)^2 \times \begin{vmatrix} 1 & 1 & 1 \\ 1/4 & -1/4 & 0 \\ 1/8 & 1/8 & -1/4 \end{vmatrix} = \frac{6}{32}$$

Then :

$$\begin{aligned} 1. \quad A(a'^4)(b''^3c'') &= \frac{4!3!6^4}{32^4} \overline{\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)\left(\frac{s}{c}\right)} \\ 2. \quad A(a'^2b'c')(b''^3c'') &= \frac{2!3!6^4}{32^4} \overline{\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)\left(\frac{s}{c}\right)\left(\frac{s}{b}\right)} \\ &= -2 \frac{2!3!6^4}{32^4} \overline{\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)} \quad *) \\ 3. \quad A(a'^2b'c')(a''^2b''^2) &= \frac{2!2!2!6^4}{32^4} \overline{\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)\left(\frac{s}{a}\right)\left(\frac{s}{a}\right)} \\ &= 3 \frac{2!2!2!6^4}{32^4} \overline{\left(\frac{s}{b}\right)\left(\frac{s}{a}\right)\left(\frac{s}{b}\right)\left(\frac{s}{c}\right)} \\ 4. \quad A(b'^2c'^2)(a''^2b''^2) &= \frac{2!2!2!2!6^4}{32^4} \overline{\left(\frac{s}{b}\right)\left(\frac{s}{a}\right)\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)} \\ &= \frac{2^4 6^4}{32^4} \overline{\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)} \end{aligned}$$

*)

The $(-)$ sign appears because we interchange the states b and c in the fourth column, and the factor 2 because :

$$\overline{\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)\left(\frac{s}{c}\right)\left(\frac{s}{b}\right)}$$

is the sum of 12 terms, while :

$$\overline{\left(\frac{s}{b}\right)\left(\frac{s}{a}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)}$$

is the sum of 6 terms.

Finally we have :

$$\psi_{2^+}^{C^{12}} \propto \overline{6 \left(\frac{s}{a} \right) \left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right)} - \overline{\left(\frac{s}{b} \right) \left(\frac{s}{a} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right)}$$

Normalizing we have :

$$\psi_{2^+ \text{ normalised}}^{C^{12}} = \frac{1}{\sqrt{42}} \left\{ 3 \overline{\left(\frac{s}{a} \right) \left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right)} - \overline{\left(\frac{s}{b} \right) \left(\frac{s}{a} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right)} \right\}^*)$$

c) $3/2$ State of N^{15} :

As a final example we shall find the wave function of the $3/2$ ground state of N^{15} when it is expressed as C^{12} oscillating against a triton.

The wave function for this state can be written immediately if we consider the $3/2$ state of N^{15} as the ground state of O^{16} with a proton hole with spin and angular momentum parallel. However, we use the above method in this case as a simple illustration only. The polynomial part of the N^{15} ground state wave function is of 11^{th} degree, while that of C^{12} is of 8^{th} degree, and the triton is in $1s$ state with 0 degree. Therefore the relative oscillation must be either $(3,1)$ or $(3,3)$ oscillation.

The spin of the triton is $\frac{1}{2}$ and if we take C^{12} in 0^+ state, we have to take the $(3,1)$ oscillation, in order to obtain total angular momentum $3/2$ in N^{15} .

*) Here a, b, c are normalized, i.e. $a = \left(\frac{\alpha}{n} \right)^{3/4} \sqrt{2} \alpha \cdot z$ etc.

We take also $J_z = 3/2$. Then :

$$\psi^{N^{15}} \propto F(c^{12})_{3s} f_{1s}(H^3) X(c^{12} - H^3)_{3,1} \quad (17)$$

In (17) we retain the term of highest degree in the polynomial part (for reasons previously explained). Now we must antisymmetrize :

$$\frac{c^{12}}{0+} \frac{X_{31}}{(b'c'+a'^2)^2 (b''c''+a''^2)^2 (b'''c''' + a'''^2 b''')} \quad (17a)$$

where

$$b' = \frac{b_1+b_2+b_3+b_4}{4} - \frac{b_5+b_6+b_7+b_8}{4}$$

similarly for a' and c'

$$b'' = \frac{b_1+\dots+b_8}{8} - \frac{b_9+b_{10}+b_{11}+b_{12}}{4}$$

similarly for c'' and a''

$$b''' = \frac{b_1+\dots+b_{12}}{12} - \frac{b_{13}+b_{15}+b_{16}}{3}$$

similarly for c''' and a''' .

Note that the number 14 which corresponds to a proton with spin "down" is missing. This is because in the H^3 we have a

single proton with spin "up". Therefore we have :

$$n_1 = n_3 = n_4 = 4 \quad \text{and} \quad n_2 = 3$$

If we expand (17), all the terms which have at least one of the a , b , or c in higher than 4th degree will vanish, as they have at least in one column two or more identical states in their antisymmetrized expressions. The remaining terms are :

$$\begin{aligned} & (b'^2 c'^2)(a''^4)(b'''^2 c''') + 2(b'^2 c'^2)(a''^2 b'' c'')(a'''^2 b''') + \\ & + 4(b' c' a'^2)(a''^2 b'' c'')(b'''^2 c''') + 2(b' c' a'^2)(b''^2 c''^2)(a'''^2 b''') + \\ & + (a'^4)(b''^2 c''^2)(b'''^2 c''') \end{aligned} \quad (17a)$$

We find that all the Q_1 , Q_3 and Q_4 are equal to $\frac{5}{2^6}$ while all the Q_2 are equal to $\frac{6}{3^2}$. Therefore for every term, the product $Q_1^i Q_2^j Q_3^k Q_4^l$ is the same = $\frac{3 \cdot 5}{2^{10}}$ and we can neglect it.

Then we obtain :

$$A(b'^2 c'^2)(a''^4)(b'''^2 c''') \propto 3 \cdot 2! \cdot 3 \cdot 4! \cdot \begin{pmatrix} s \\ a \\ c \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ b \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix}$$

$$A(b'^2 c'^2)(a''^2 b'' c'')(a'''^2 b''') \propto 2! \cdot 4 \cdot 6 \cdot \begin{pmatrix} s \\ a \\ c \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ b \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix}$$

$$A(b' c' a'^2)(a''^2 b'' c'')(b'''^2 c''') \propto 2! \cdot 3 \cdot 12 \cdot \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ b \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix}$$

$$A(b' c' a'^2)(b''^2 c''^2)(a'''^2 b''') \propto 2! \cdot 4 \cdot 6 \cdot \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ b \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix}$$

$$A(a'^4)(b''^2 c''^2)(b'''^2 c''') \propto 3! \cdot 2 \cdot 3 \cdot 4! \cdot \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ b \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix}$$

Therefore the antisymmetrized wave function of N^{15} for $3/2$ state is a single determinant

$$\psi_{3/2}^{N^{15}} = \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} \begin{pmatrix} s \\ a \\ b \\ c \end{pmatrix} .$$

III. Antisymmetrization for Cluster Model wave functions:

As we mentioned before, the method which is given in Part II is not easily applicable to nuclei with particles occupying states higher than the 1p-shell. In the present chapter, we give a more general method in which we can obtain antisymmetrized wave functions for any nucleus, provided its cluster structure is given.

Here we again suppose that we have harmonic oscillator wave functions.

In the Cluster Model, a nucleus can be represented as two clusters ^{*)} oscillating against each other. Each of the clusters is in a definite state and its wave function can be taken antisymmetrized. Therefore the problem is to antisymmetrize expressions of the form :

$$f_1(1,2,\dots,n) f_2(n+1,\dots,N) X(\underline{R}_1 - \underline{R}_2) \quad (18)$$

where f_1 and f_2 are the antisymmetric wave functions of the two clusters, and X is the wave function of their relative motion with :

$$\begin{aligned} \underline{R}_1 &= \frac{\sum_{i=1}^n \underline{r}_i}{n} \\ \underline{R}_2 &= \frac{\sum_{j=n+1}^N \underline{r}_j}{N-n} \end{aligned}$$

^{*)} If there are more than two clusters, we can combine the small clusters in bigger and bigger ones, in order to obtain finally only two clusters.

As previously, for the antisymmetrization of (18), we omit the exponential part which is symmetric in all the particles, and we just have to antisymmetrize the polynomial part of (18).

The polynomial part X' of $X(R_1-R_2)$ has a definite degree n' and it is a sum of homogeneous polynomials in x, y, z , from n' to 0 or 1 degree (for n' even or odd respectively). From these parts of X' it is usually enough to take into account only the part of the highest degree n' . It will be necessary to take the next one, which is of $n'-2$, when there are many unoccupied states in either or both of the wave functions f_1 and f_2 below the highest occupied one.

It is again convenient to put :

$$\begin{aligned} z &= a \\ x + iy &= b \\ x - iy &= c \end{aligned}$$

and express the polynomial X' (or the highest part of it) in terms of a, b, c .

Then from X' we take the terms :

$$\sum_{k, \ell, m} a^k b^\ell c^m \quad (19)$$

(with $k+\ell+m = n'$ and if necessary $k+\ell+m = n'-2$ etc.)

where here :

$$\begin{aligned} a &= \frac{a_1 + a_2 + \dots + a_n}{n} - \frac{a_{n+1} + \dots + a_N}{N-n} \\ b &= \frac{b_1 + b_2 + \dots + b_n}{n} - \frac{b_{n+1} + \dots + b_N}{N-n} \\ c &= \frac{c_1 + c_2 + \dots + c_n}{n} - \frac{c_{n+1} + \dots + c_N}{N-n} \end{aligned} \quad (20)$$

The antisymmetrization of (18) is based on the results of §§ iv and vii of Part I.

The f_1 and f_2 in (18) are combinations of Slater determinants, with no common particles. If $X'(\underline{R}_1, -\underline{R}_2)$ was a constant, i.e. if $X(\underline{R}_1, -\underline{R}_2)$ is a 1s oscillation, then the antisymmetric expression of (18) is, according to (iv, I), a determinant whose principal diagonal is the "sum" of the diagonals of the determinants for f_1 and f_2 . If there exists at least one common state in the two Slater determinants, which are joined together, the total determinant vanishes. Usually $X'(\underline{R}_1, -\underline{R}_2)$ is not a constant. Then it can be written, using (19) and (20), as a sum of terms of the form $a_i^l b_i^m c_i^n$. Using (§vii, I), we can insert this form into the determinants for the clusters 1 and 2, obtaining thus products of Slater determinants with no common particles. The final step is to join the diagonals in each product to obtain the antisymmetric expression for each term.

The number of the terms is rather large in every expression (18), when using (19) and (10) we write it as a sum of monomials in $a_i b_i c_i$ and it increases very rapidly when the clusters become larger. However, we can find out from the beginning which of the terms of $X(\underline{R}_1, -\underline{R}_2)$ contribute to the final result. Looking at the Slater determinants for the two clusters, we see that there are many common states. The effect of the $X(\underline{R}_1, -\underline{R}_2)$ part must be such that in the final determinant there are no two particles in the same state, therefore it has to be used to shift at least the states which are common in the two partial Slater determinants.

We give some examples below, in order to illustrate the method. Several abbreviations can be used and especially we shall see that the explicit expansion of (19) in terms of (20) can be avoided.

Examples :

As examples, we shall construct the wave functions for the 1^- , 2^- , and 3^- states of O^{16} .

1) 1^- state

We can consider the following cases ^{*)} :

$$\begin{aligned}
 \alpha) \quad \psi &= (C^{12})_{3s} \quad f_{1s}(\alpha) \quad X_{(5,1)}(\underline{R}_1 - \underline{R}_2) \\
 \beta) \quad \psi &= (C^{12})_{2D} \quad f_{1s}(\alpha) \quad X_{(5,1)}(\underline{R}_1 - \underline{R}_2) \\
 \gamma) \quad \psi &= (C^{12})_{2D} \quad f_{1s}(\alpha) \quad X_{(5,3)}(\underline{R}_1 - \underline{R}_2) \\
 \delta) \quad \psi &= (C^{12})_{1G} \quad f_{1s}(\alpha) \quad X_{(5,3)}(\underline{R}_1 - \underline{R}_2) \\
 \epsilon) \quad \psi &= (C^{12})_{1G} \quad f_{1s}(\alpha) \quad X_{(5,5)}(\underline{R}_1 - \underline{R}_2)
 \end{aligned}
 \quad \begin{aligned}
 \underline{R}_1 &= \frac{\underline{r}_1 + \dots + \underline{r}_{12}}{12} \\
 \underline{R}_2 &= \frac{\underline{r}_{13} + \dots + \underline{r}_{16}}{4}
 \end{aligned}$$

We find that all the cases except (γ) give the same result. For (γ) we find that it is identically zero. We shall give here in detail only case α).

The un-normalized $3s$ wave function of C^{12} with $s=1$, $z=a$, $x+iy=b$ and $x-iy=c$ is :

$$(C^{12})_{3s} = 3 \overline{\left(\frac{s}{c} \right) \left(\frac{s}{c} \right) \left(\frac{s}{c} \right) \left(\frac{s}{c} \right)} - 2 \overline{\left(\frac{s}{c} \right) \left(\frac{s}{c} \right) \left(\frac{s}{c} \right) \left(\frac{s}{b} \right)} - 8 \overline{\left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right) \left(\frac{s}{c} \right)},$$

where the bar indicates that we have to take the sum of the

^{*)} Here $X(n, \ell)(\underline{R})$ denotes oscillation with principal quantum number n and angular momentum ℓ .

different permutations among the columns.

$$f(\alpha) = (s) (s) (s) (s)$$

and

$$X_{51} = b'^3 c'^2 + 2a'^2 b'^2 c' + a'^4 b'$$

with

$$b' = \frac{b_1 + b_2 + \dots + b_{12}}{12} - \frac{b_{13} + \dots + b_{16}}{4}$$

and similarly for a' and c' .

We take :

$$1) Q_1 = \left(\frac{s}{c}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right) (ssss) (b'^3 c'^2 + 2a'^2 b'^2 c' + a'^4 b') \quad (1)$$

We have to use the terms of the expansion in the brackets to shift at least 4 particles from the 1s states from either cluster

(i) from $b'^3 c'^2$ we get 0	} coefficient $\frac{24}{4 \cdot 3^5}$	because there will be in one of the columns, at least twice the same state b or c
(ii) from $2a'^2 b'^2 c'$ again 0		
(iii) from $a'^4 b' \rightarrow aaaa.b \rightarrow \overline{aaaa}$ $aaab.a \rightarrow \overline{aaab}$ $aaa(ab) \rightarrow \overline{aaa(ab)}$		

Therefore :

$$\begin{aligned}
 AQ_1 &= \frac{4!}{4 \cdot 3^5} \left\{ \overline{\begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ bc \end{pmatrix}} - \overline{\begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ b2 \end{pmatrix}} - 3 \overline{\begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \begin{pmatrix} s \\ ab \end{pmatrix}} \right\} = \\
 &= \frac{4!}{4 \cdot 3^5} \left\{ \overline{\begin{pmatrix} s \\ bc \end{pmatrix}} - \overline{\begin{pmatrix} s \\ b2 \end{pmatrix}} - 3 \overline{\begin{pmatrix} s \\ ab \end{pmatrix}} \right\} \quad *)
 \end{aligned}$$

Note: In order to find the coefficients we keep in mind that for the first cluster the coefficients are all equal to $1/12$ and for the second $-1/4$. The term $aaaa.b$ means that the four a 's will occupy the s states from either cluster and the b will be combined with one of the other states of the first cluster only. The b for any column gives the factor $1/12$. For the a 's we see that in every column they can occupy the s state, either from the first or the second cluster. For the first cluster give $1/12$ and for the second $-1/4$, but exchanging the order in the last, we have to change the sign. So finally for every a -state we obtain a coefficient $1/12 + 1/4 = 1/3$. The total coefficient will then be :

$$\left(\frac{1}{3}\right)^4 \times \frac{1}{12} = \frac{1}{4 \cdot 3^5}$$

which has to be multiplied by $4 !$

*) Here from the four columns, we write only the one which differs from

$$\begin{pmatrix} s \\ c \\ c \\ c \end{pmatrix}$$

Now for $aaa(ab)$ in a similar way we obtain the coefficient :

$$\frac{1}{3} \times \frac{1}{3} \times \frac{1}{3} \times \left(\frac{1}{12^2} - \frac{1}{4^2} \right) = \frac{2}{4 \cdot 3^5}$$

$$Q_2 = \overline{\left(\frac{s}{a} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right) \left(\frac{s}{b} \right)} (ssss) (b'^3 c'^2 + 2a'^2 b'^2 c' + a'^4 b') \quad (2)$$

(i) from $b'^3 c'^2$ we get 0

$$\begin{array}{lcl} \text{(ii) from } 2a'^2 b'^2 c' : aabb.c & \rightarrow & \begin{array}{c} baab \\ c \end{array} \\ aabc.b & \rightarrow & \begin{array}{c} baac + baac + baac + baac \\ b \quad b \quad b \quad b \end{array} \\ abbc.a & \rightarrow & \begin{array}{c} babc + bbac \\ a \quad a \end{array} \end{array} \left. \vphantom{\begin{array}{l} aabc.b \\ abbc.a \end{array}} \right\} \begin{array}{l} \text{Coefficient} \\ \frac{8}{4 \cdot 3^5} \end{array}$$

$$\begin{array}{lcl} a^2bbc & \rightarrow & 0 \\ aab^2c & \rightarrow & b^2aac \end{array} \left. \vphantom{\begin{array}{l} a^2bbc \\ aab^2c \end{array}} \right\} \begin{array}{l} \text{Coefficient} \\ - \frac{8}{4 \cdot 3^5} \end{array}$$

$$\begin{array}{lcl} aab(bc) & \rightarrow & baa(bc) \\ abc(ab) & \rightarrow & ba(ab)c + b(ab)ac \\ abb(ac) & \rightarrow & 0 \end{array} \left. \vphantom{\begin{array}{l} aab(bc) \\ abc(ab) \\ abb(ac) \end{array}} \right\} \begin{array}{l} \text{Coefficient} \\ - \frac{16}{4 \cdot 3^5} \end{array}$$

From which we obtain :

$$(ii) = - \frac{24}{4 \cdot 3^5} \left\{ 2 \overline{\left(\frac{s}{a} \right) \left(\frac{s}{c} \right)^2} + 4 \overline{\left(\frac{s}{b} \right) \left(\frac{s}{ab} \right)} \right\}$$

(iii) From $a'^4 b'$:

$$\begin{array}{lcl} aaaa.b & \rightarrow & 0 \\ aaab.a & \rightarrow & \begin{array}{c} baaa \\ a \end{array} \\ a^2aab & \rightarrow & baaa^2 \\ aaa(ab) & \rightarrow & 0 \end{array} \left. \vphantom{\begin{array}{l} aaaa.b \\ aaab.a \\ a^2aab \\ aaa(ab) \end{array}} \right\} \begin{array}{l} \text{Coefficient} \\ \frac{24}{4 \cdot 3^5} \\ - \frac{24}{4 \cdot 3^5} \end{array}$$

Therefore :

$$(iii) = - \frac{48.3}{4.3^5} \left(\overline{\begin{smallmatrix} s & s \\ b & b \\ a^2 \end{smallmatrix}} \right)$$

Combining (i), (ii) and (iii), we have :

$$Q_2 = - \frac{48}{4.3^5} \left\{ 3 \left(\overline{\begin{smallmatrix} s & s \\ b & b \\ a^2 \end{smallmatrix}} \right) + \left(\overline{\begin{smallmatrix} s & s \\ c & c \\ b^2 \end{smallmatrix}} \right) + 2 \left(\overline{\begin{smallmatrix} s & s \\ c & c \\ a b \end{smallmatrix}} \right) \right\}$$

Finally :

$$3/ \quad Q_3 = \overline{\left(\begin{smallmatrix} s \\ a \end{smallmatrix} \right) \left(\begin{smallmatrix} s \\ b \end{smallmatrix} \right) \left(\begin{smallmatrix} s \\ c \end{smallmatrix} \right) \left(\begin{smallmatrix} s \\ a \end{smallmatrix} \right)} \cdot (ssss) \quad (b'^3 c'^2 + 2a'^2 b'^2 c' + a'^4 b')$$

(i) From $b'^3 c'^2$:

$$\begin{array}{ll} bbbc.c \rightarrow \begin{matrix} bbbb & cbbb \\ c & c \end{matrix} \\ bbcc.b \rightarrow \begin{matrix} ccbb & ccbb & ccbb & ccbb \\ b & b & b & b \end{matrix} \end{array} \left. \vphantom{\begin{array}{l} bbbc.c \\ bbcc.b \end{array}} \right\} \begin{array}{l} \text{Coefficients} \\ \frac{12}{4.3^5} \end{array}$$

$$\begin{array}{ll} b^2bcc \rightarrow ccb^2b + ccbb^2 \\ bbbc^2 \rightarrow 0 \\ bbc(bc) \rightarrow c(bc)bb + (bc)cbb \end{array} \left. \vphantom{\begin{array}{l} b^2bcc \\ bbbc^2 \\ bbc(bc) \end{array}} \right\} \begin{array}{l} \text{Coefficient} \\ - \frac{24}{4.3^5} \end{array}$$

$$(i) = \frac{72}{4.3^5} \left\{ \left(\overline{\begin{smallmatrix} s \\ b \\ c \\ ab \end{smallmatrix}} \right) - \left(\overline{\begin{smallmatrix} s \\ b \\ c \\ bc \end{smallmatrix}} \right) \right\}$$

$$(ii) 2a'^2 b'^2 c' :$$

$$\left. \begin{array}{l} aabb.c \rightarrow 0 \\ aabc.b \rightarrow 0 \\ bbca.a \rightarrow \frac{acbb}{a} + \frac{cabb}{a} \end{array} \right\} \times \frac{8}{4 \cdot 3^5}$$

$$\left. \begin{array}{l} a^2bbc \rightarrow a^2cbb + ca^2bb \\ ab^2ac \rightarrow 0 \\ bba(ac) \rightarrow 0 \end{array} \right\} \times -\frac{8}{4 \cdot 3^5}$$

$$(ii) = -\frac{48}{4 \cdot 3^5} \left(\overline{\begin{pmatrix} s \\ a \\ b \\ a^2 \end{pmatrix}} \right)$$

$$(iii) a'^4 b' \rightarrow 0 \quad \text{and}$$

$$Q_3 = \frac{24}{4 \cdot 3^5} \left\{ 3 \left(\overline{\begin{pmatrix} s \\ b \\ c \\ ab \end{pmatrix}} \right) - 3 \left(\overline{\begin{pmatrix} s \\ a \\ b \\ bc \end{pmatrix}} \right) - 2 \left(\overline{\begin{pmatrix} s \\ a \\ b \\ a^2 \end{pmatrix}} \right) \right\}$$

Then :

$$\psi^1 \propto 3 \left(\overline{\begin{pmatrix} s \\ a \\ b \\ bc \end{pmatrix}} \right) + \left(\overline{\begin{pmatrix} s \\ a \\ c \\ b^2 \end{pmatrix}} \right) - \left(\overline{\begin{pmatrix} s \\ b \\ c \\ ab \end{pmatrix}} \right) + 4 \left(\overline{\begin{pmatrix} s \\ a \\ b \\ a^2 \end{pmatrix}} \right) \quad (21)$$

Putting now :

$$\begin{aligned} d &= (x+iy)^2 \propto d(2,2) & g &= z(x-iy) \propto d(2,-1) \\ f &= z(x+iy) \propto d(2,1) & e &= (x-iy)^2 \propto d(2,-2) \\ h &= 2z^2 - x^2 - y^2 \propto d(2,0) & i &= \frac{3}{\alpha} - 2r^2 \propto 2s \end{aligned}$$

we find :

$$\psi^{1-} \propto \frac{1}{3} \begin{pmatrix} \bar{s} \\ \bar{s} \\ \bar{b} \\ \bar{b} \\ \bar{h} \end{pmatrix} - \frac{5}{3} \begin{pmatrix} \bar{s} \\ \bar{s} \\ \bar{b} \\ \bar{b} \\ \bar{1} \end{pmatrix} + \begin{pmatrix} \bar{s} \\ \bar{s} \\ \bar{c} \\ \bar{c} \\ \bar{d} \end{pmatrix} - \begin{pmatrix} \bar{s} \\ \bar{s} \\ \bar{b} \\ \bar{b} \\ \bar{1} \end{pmatrix}$$

Using the same notation for the normalized functions a, b, c etc., we have for the normalized wave function :

$$\psi_{\text{normalized}}^{1-} = \frac{1}{12\sqrt{5}} \left\{ \sqrt{3} \begin{pmatrix} \bar{s} \\ \bar{s} \\ \bar{b} \\ \bar{b} \\ \bar{h} \end{pmatrix} - 5\sqrt{6} \begin{pmatrix} \bar{s} \\ \bar{s} \\ \bar{b} \\ \bar{b} \\ \bar{1} \end{pmatrix} + 3\sqrt{2} \begin{pmatrix} \bar{s} \\ \bar{s} \\ \bar{c} \\ \bar{c} \\ \bar{d} \end{pmatrix} - 3 \begin{pmatrix} \bar{s} \\ \bar{s} \\ \bar{b} \\ \bar{b} \\ \bar{1} \end{pmatrix} \right\} \quad (22)$$

2) 2^- State of O^{16} :

Clustering into C^{12} and an α -particle, we can obtain the 2^- state of O^{16} from either of the following cases :

$$\alpha) (C^{12})_{2D} f_{1s}(\alpha) X_{(5,1)}(\underline{R}_1 - \underline{R}_2)$$

$$\beta) (C^{12})_{2D} f_{1s}(\alpha) X_{(5,3)}(\underline{R}_1 - \underline{R}_2)$$

$$\gamma) (C^{12})_{1G} f_{1s}(\alpha) X_{(5,3)}(\underline{R}_1 - \underline{R}_2)$$

$$\delta) (C^{12})_{1G} f_{1s}(\alpha) X_{(5,5)}(\underline{R}_1 - \underline{R}_2)$$

All the cases lead to the same result. We shall consider here only the case α).

We find that, taking a , b , and c unnormalized :

$$\psi^{2-} \propto 4 \left\{ \overline{6 \left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right)} - \overline{\left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right) \left(\frac{s}{c} \right)} \right\} (ssss) (a' b'^2 c'^2 + 2a' b'^3 c' + a'^5) +$$

$$+ \left\{ \overline{3 \left(\frac{s}{c} \right) \left(\frac{s}{c} \right) \left(\frac{s}{b} \right) \left(\frac{s}{b} \right)} - \overline{4 \left(\frac{s}{c} \right) \left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{b} \right)} \right\} (ssss) [b'^3 c'^2 + 2a' b'^2 c' + a' b'^4]$$

$$(1) \quad \overline{\left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right)} :$$

$$a' b'^2 c'^2 \rightarrow \frac{48}{4 \cdot 3^5} \overline{\left(\frac{s}{a} \right) \left(\frac{s}{b} \right) \left(\frac{s}{ab} \right)}$$

$$2a' b'^3 c' \rightarrow 0$$

$$a'^5 \rightarrow 0$$

$$(2) \quad \overline{\left(\frac{s}{b} \right) \left(\frac{s}{b} \right) \left(\frac{s}{c} \right) \left(\frac{s}{c} \right)} :$$

$$a' b'^2 c'^2 \rightarrow -\frac{24}{4 \cdot 3^5} \overline{\left(\frac{s}{c} \right) \left(\frac{s}{c^2} \right) \left(\frac{s}{b^2} \right)}$$

$$2a' b'^3 c' \rightarrow -\frac{12^2}{4 \cdot 3^5} \overline{\left(\frac{s}{a} \right) \left(\frac{s}{b} \right) \left(\frac{s}{ab} \right)}$$

$$a'^5 \rightarrow 0$$

(3)

$$\overline{\left(\frac{s}{b}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)\left(\frac{s}{b}\right)} :$$

$$\begin{aligned} b'3c'2 &\rightarrow 0 \\ 2a'2b'2c' &\rightarrow -\frac{48}{4 \cdot 3^5} \overline{\left(\frac{s}{b} \frac{s}{c} \frac{s}{c} \frac{s}{b}\right)} \\ a'4b' &\rightarrow -\frac{96}{4 \cdot 3^5} \overline{\left(\frac{s}{a} \frac{s}{b} \frac{s}{b} \frac{s}{a}\right)} \end{aligned}$$

(4)

$$\overline{\left(\frac{s}{b}\right)\left(\frac{s}{a}\right)\left(\frac{s}{b}\right)\left(\frac{s}{a}\right)} :$$

$$\begin{aligned} b'3c'2 &\rightarrow \frac{72}{4 \cdot 3^5} \overline{\left(\frac{s}{b} \frac{s}{c} \frac{s}{c} \frac{s}{b}\right)} \\ 2a'2b'c' &\rightarrow \frac{24 \times 8}{4 \cdot 3^5} \overline{\left(\frac{s}{a} \frac{s}{b} \frac{s}{c} \frac{s}{a}\right)} \\ a'4b' &\rightarrow 0 \end{aligned}$$

Therefore :

$$\psi_{\text{unnormalized}}^{2-} \propto 2 \overline{\left(\frac{s}{a} \frac{s}{b}\right)} - \overline{\left(\frac{s}{b} \frac{s}{c} \frac{s}{c} \frac{s}{b}\right)}$$

and for normalised a, b, c, etc.

$$\psi_{\text{normalised}}^{2-} = \frac{1}{6} \left[\overline{\left(\frac{s}{a} \frac{s}{b}\right)} - 2\sqrt{2} \overline{\left(\frac{s}{b} \frac{s}{c} \frac{s}{c} \frac{s}{b}\right)} \right]$$

3) 3⁻ State of 0¹⁶ :

We have six different combinations of C¹² in 3s, 2D or 1G state and relative oscillation against α-particle X₅₁, X₅₃ or X₅₅. All lead to the same final result. Taking the combi-

nation, for example :

$$(c^{12})_{3s} f_{1s}(\alpha) X_{53}(\underline{R}_1 - \underline{R}_2)$$

we have :

$$\begin{aligned} \psi^{3-} &\propto \left\{ 3 \overline{\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)} - 2 \overline{\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)\left(\frac{s}{b}\right)} + 8 \overline{\left(\frac{s}{b}\right)\left(\frac{s}{b}\right)\left(\frac{s}{c}\right)\left(\frac{s}{c}\right)} \right\} c^{12} \times \\ &\times (ssss)_{\alpha} \times \int b'^4 c'^2 a'^2 b'^3 \int_{X_{53}} \end{aligned}$$

We see at once that the only non-vanishing term we can obtain is :

$$\psi^{3-} = \overline{\left(\frac{ssss}{c}\right)\left(\frac{ssss}{c}\right)\left(\frac{ssss}{c}\right)\left(\frac{ssss}{b^2}\right)}$$

IV. General considerations on Antisymmetrisation (or Symmetrisation)

1. Suppose we have to antisymmetrise (symmetrise) the function $f(x_1, x_2, \dots, x_n)$ with respect to all coordinates x_i .

We write :

$$f(x_1, x_2, \dots, x_n) = \int f(x'_1, x'_2, \dots, x'_n) \delta(x_1 - x'_1) \delta(x_2 - x'_2) \dots \delta(x_n - x'_n) d\tau'_1 \dots d\tau'_n \quad (22)$$

where x_i and $d\tau'_i$ are extended to include spin and i-spin coordinates. If A and S are the operators for antisymmetrisation or symmetrisation, we have:

$$Af(x_1, \dots, x_n) = \frac{1}{n!} \int f(x'_1, \dots, x'_n) \begin{vmatrix} \delta(x_1 - x'_1) & \delta(x_1 - x'_2) & \dots & \delta(x_1 - x'_n) \\ \delta(x_2 - x'_1) & \delta(x_2 - x'_2) & \dots & \delta(x_2 - x'_n) \\ \vdots & \vdots & \ddots & \vdots \\ \delta(x_n - x'_1) & \delta(x_n - x'_2) & \dots & \delta(x_n - x'_n) \end{vmatrix} d\tau'_1 \dots d\tau'_n \quad (22a)^{(*)}$$

or

$$Sf(x_1, \dots, x_n) = \frac{1}{n!} \int f(x'_1, \dots, x'_n) \begin{bmatrix} \delta(x_1 - x'_1) & \dots & \delta(x_1 - x'_n) \\ \vdots & \ddots & \vdots \\ \delta(x_n - x'_1) & \dots & \delta(x_n - x'_n) \end{bmatrix} d\tau'_1 \dots d\tau'_n \quad (22b)$$

where $\begin{bmatrix} \end{bmatrix}$ denotes the permanent of $\delta(x_i - x'_j)$'s.

If in (22a) $f(x_1 \dots x_n)$ is already antisymmetrised we have

$$Af(x_1 \dots x_n) = f(x_1 \dots x_n)$$

or $A^2 = A$

The same for (22b)

$$S(Sf) = Sf \quad \text{or} \quad S^2 = S$$

(*) This expression of antisymmetric wave functions is already used in reference 2.

$$= \frac{\ell!(n-\ell)!}{n!} (-)^{\frac{\ell(\ell+1)}{2}} \sum_{n\zeta_e}^{[\zeta_e]} (-)^{A(k, \dots, j)} f(x_k, \dots, x_m; x_k, \dots, x_j) \quad (23a)$$

When $f(x_1 \dots x_\ell, x_{\ell+1} \dots x_n)$ is antisymmetric separately for the first ℓ and the other $n-\ell$ variables, then

$$Af = \frac{\ell!(n-\ell)!}{n!} (-)^{\frac{\ell(\ell+1)}{2}} \sum_{n\zeta_e}^{[\zeta_e]} (-)^{A(i_1, i_2, \dots, i_\ell; i_{\ell+1}, \dots, i_n)} f(x_{i_1}, x_{i_2}, \dots, x_{i_\ell}; x_{i_{\ell+1}}, \dots, x_{i_n}) \quad (23b)$$

- (iiia) If $f(x_1 \dots x_\ell; x_{\ell+1} \dots x_n)$ is symmetric with respect to the ℓ first variables and we want to symmetrise it on the whole, we get, in a similar way,

$$Sf(x_1 \dots x_\ell, x_{\ell+1} \dots x_n) = \frac{\ell!(n-\ell)!}{n!} \sum_{n\zeta_e} S(i_1, \dots, i_\ell) f(x_{i_1}, x_{i_2}, \dots, x_{i_\ell}; x_{i_{\ell+1}}, \dots, x_{i_n}) \quad (23c)$$

Also if $f(x_1 \dots x_\ell, x_{\ell+1} \dots x_n)$ is symmetric separately for the first ℓ and the other $n-\ell$ variables, then :

$$Sf(x_1 \dots x_\ell, x_{\ell+1} \dots x_n) = \frac{(n-\ell)! \ell!}{n!} \sum_{n\zeta_e} f(x_{i_1}, x_{i_2}, \dots, x_{i_\ell}; x_{i_{\ell+1}}, \dots, x_{i_n}) \quad (23d)$$

- (iv) If $f(x_1 \dots x_n) = u(x_1 \dots x_n) \cdot v(x_1 \dots x_n)$ and $u(x_i)$ is already antisymmetric, then

$$Af(x_1 \dots x_n) = u(x_1 \dots x_n) \cdot [S v(x_1 \dots x_n)] \quad (24)$$

Also if $u(x_i)$ is already symmetric, then

$$Sf(x_1 \dots x_n) = u(x_1 \dots x_n) [Sv(x_1 \dots x_n)] \quad (24)$$

- (v) It is easy to verify, using (22a) and (22b), that

$$\begin{aligned} (Au) \cdot (Av) &= S [u(Av)] = S [v(Au)] \\ (Au) \cdot (Sv) &= A [u(Sv)] = A [v(Au)] \end{aligned} \quad (25)$$

Therefore the expressions :

$$u(SV) \quad \text{and} \quad v(Au)$$

after antisymmetrisation lead to the same result.

Also

$$(Su) (Sv) = S[u(Sv)] = S[v(Su)] \quad (25a)$$

(vi) If $f = u(x_1 \dots x_{\ell}, x_{\ell+1} \dots x_n) \cdot v(x_1 \dots x_{\ell})$ then

$$Af = \frac{\ell!(n-\ell)!}{n!} \sum_{\eta \zeta_{\ell}} (-)^{[\zeta_{\ell}]} A(i_1 \dots i_{\ell}) \{ v(x_{i_1} \dots x_{i_{\ell}}) A(i_{\ell+1} \dots i_n) u(x_{i_1}, x_{i_2} \dots x_{i_n}) \} \quad (26a)$$

and if u is a function of $x_{\ell+1} \dots x_n$ only

$$Af = \frac{\ell!(n-\ell)!}{n!} \sum_{\eta \zeta_{\ell}} (-)^{[\zeta_{\ell}]} (Au)(Av) \quad (26b)$$

(vii) We can always write :

$$A(1, 2, \dots, n) = \frac{\ell!(n-\ell)!}{n!} \sum_{\eta \zeta_{\ell}} (-)^{[\zeta_{\ell}]} A(i_1 \dots i_{\ell}) A(i_{\ell+1} \dots i_n) \quad (27)$$

and

$$S(1, 2, \dots, n) = \frac{\ell!(n-\ell)!}{n!} \sum_{\eta \zeta_{\ell}} S(i_1, i_2, \dots, i_{\ell}) S(i_{\ell+1}, \dots, i_n) \quad (27a)$$

Then if we have

$$f = u(x_1 \dots x_{\ell}) \cdot v(x_{\ell+1} \dots x_n) \cdot X(x_1, \dots, x_{\ell}, x_{\ell+1}, \dots, x_n) \quad (28)$$

where u and v are already antisymmetric while X is symmetric separately for the first ℓ and the last $n-\ell$ variables, then

$$\begin{aligned} Af &= \frac{\ell!(n-\ell)!}{n!} \sum_{\eta \zeta_{\ell}} (-)^{[\zeta_{\ell}]} A(i_1 \dots i_{\ell}) A(i_{\ell+1} \dots i_n) u \cdot v \cdot X = \\ &= \frac{\ell!(n-\ell)!}{n!} \sum_{\eta \zeta_{\ell}} (-)^{[\zeta_{\ell}]} u(x_{i_1} \dots x_{i_{\ell}}) v(x_{i_{\ell+1}} \dots x_{i_n}) X(x_{i_1} \dots x_{i_{\ell}}, x_{i_{\ell+1}} \dots x_{i_n}) \end{aligned} \quad (28a)$$

This is the case for Cluster Model wave functions in a general form. For harmonic oscillator wave functions it reduces to the case with which we deal in Part III.

2. The matrix element of an Operator $O(1, \dots, n)$ is given by :

$$O_{ij} = \frac{1}{N_i N_j} \int (A f_i)^* O (A f_j) d\tau_1 \dots d\tau_n \quad (29)$$

where $\frac{1}{N_i}$ the normalisation factor of $(A f_i)$

When O is symmetric in all particles, then^{*})

$$O_{ij} = \frac{1}{N_i N_j} \int f_i^*(1, 2, \dots, n) O(1, 2, \dots, n) [A f_j(1, \dots, n)] d\tau_1 \dots d\tau_n \quad (29)$$

and

$$|N_i|^2 = \int f_i^*(1, \dots, n) [A f_i(1, \dots, n)] d\tau_1 \dots d\tau_n \quad (30)$$

Therefore, using (22a), we obtain :

$$O = \frac{1}{n! N_i N_j} \iint f_i^*(1, 2, \dots, n) O(1, 2, \dots, n) \cdot f_j(1', 2', \dots, n') \begin{vmatrix} \delta(1-1') \dots \delta(1-n') \\ \vdots \\ \delta(n-1') \dots \delta(n-n') \end{vmatrix} d\Omega d\Omega'$$

where $d\Omega = d\tau_1 \dots d\tau_n$

3. Suppose we have a function $f(x_1, x_2 \dots x_n)$ which is analytic in the neighbourhood of a point (ξ_i) . Then we can expand it in a Taylor series :

$$f(x_1, x_2, \dots, x_n) = \sum_{\substack{l_1, l_2, \dots, l_n = 0 \\ l_1 + l_2 + \dots + l_n = k}}^{\infty} \frac{(x_1 - \xi_1)^{l_1} (x_2 - \xi_2)^{l_2} \dots (x_n - \xi_n)^{l_n}}{l_1! l_2! \dots l_n!} \left[\frac{\partial^{(k)}}{\partial x_1^{l_1} \dots \partial x_n^{l_n}} f(x_1 \dots x_n) \right]_{x_i = \xi_i} \quad (31)$$

^{*}) Here for simplicity we write only the indices of the co-ordinates.

After antisymmetrisation we obtain :

$$Af = \frac{1}{n!} \sum_{l_p=0}^{\infty} \frac{1}{l_1! l_2! \dots l_n!} \left(\begin{matrix} (x_1 - \xi_1)^{l_1} & (x_1 - \xi_2)^{l_2} & \dots & (x_1 - \xi_n)^{l_n} \\ (x_2 - \xi_1)^{l_1} & (x_2 - \xi_2)^{l_2} & \dots & (x_2 - \xi_n)^{l_n} \\ \vdots & \vdots & \ddots & \vdots \\ (x_n - \xi_1)^{l_1} & (x_n - \xi_2)^{l_2} & \dots & (x_n - \xi_n)^{l_n} \end{matrix} \right) \left(\begin{matrix} \frac{\partial^{l_1}}{\partial x_1^{l_1}} & \frac{\partial^{l_2}}{\partial x_1^{l_2}} & \dots & \frac{\partial^{l_n}}{\partial x_1^{l_n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^{l_1}}{\partial x_n^{l_1}} & \frac{\partial^{l_2}}{\partial x_n^{l_2}} & \dots & \frac{\partial^{l_n}}{\partial x_n^{l_n}} \end{matrix} \right) f(x_i) \Big|_{x_i = \xi_i} \quad (32)$$

$$k = \sum_{p=1}^n l_p \geq \frac{n(n-1)}{2}$$

Then for every analytic function at a point (ξ_i) the operator of antisymmetrisation takes the differential form :

$$A(l, \dots, n) = \frac{1}{n!} \sum_{l_p=0}^{\infty} \frac{1}{l_1! l_2! \dots l_n!} \left(\begin{matrix} (x_1 - \xi_1)^{l_1} & (x_1 - \xi_2)^{l_2} & \dots & (x_1 - \xi_n)^{l_n} \\ (x_2 - \xi_1)^{l_1} & (x_2 - \xi_2)^{l_2} & \dots & (x_2 - \xi_n)^{l_n} \\ \vdots & \vdots & \ddots & \vdots \\ (x_n - \xi_1)^{l_1} & (x_n - \xi_2)^{l_2} & \dots & (x_n - \xi_n)^{l_n} \end{matrix} \right) \times \left(\begin{matrix} \frac{\partial^{l_1}}{\partial x_1^{l_1}} & \dots & \frac{\partial^{l_n}}{\partial x_1^{l_n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^{l_1}}{\partial x_n^{l_1}} & \dots & \frac{\partial^{l_n}}{\partial x_n^{l_n}} \end{matrix} \right) \Big|_{x_i = \xi_i} \quad (33)$$

$$\sum_{p=1}^n l_p = k \geq \frac{n(n-1)}{2}$$

The lowest derivatives of $f(x_1 \dots x_n)$ which appear in Af are of order $K = \frac{n(n-1)}{2}$. This is because for $l_1 + l_2 + \dots + l_n < \frac{n(n-1)}{2}$ the determinant of $(x_i - \xi_j)$ vanishes as one can see by expanding the elements of the determinant and splitting it in a sum of Van der Monde determinants in x_i (or ξ_j).

Suppose that a function $f(x_1 \dots x_n)$ is analytic in a domain D . Then (32) gives the value of Af at a certain point $(x_1, x_2 \dots x_n)$ as a function of the values of f and its derivatives at any point $(\xi_1, \xi_2, \dots, \xi_n)$ of the domain D .

It follows that :

Theorem:

If a function $f(x_i)$ of n variables is an analytic function in a domain D , then the antisymmetric expression of it is independent of all derivatives of $f(x_i)$ which are of order lower than $\frac{n(n-1)}{2}$.

This shows that one has to be careful in extending results obtained with a non-antisymmetrized wave function to the case where antisymmetrization is taken into account.

The above results are valid for the case in which we have n particles in one-dimensional space, without taking into account spin and i-spin. The corresponding expressions for the general case of 3-dimensional case with spin and i-spin accounted for, are

$$f(\underline{r}_1, \underline{r}_2, \dots, \underline{r}_n) = \sum_{\substack{l_1, \dots, l_n \\ j_1, \dots, j_n \\ k_1, \dots, k_n}}^{\infty} \frac{(x_1 - \xi_1)^{l_1} (\gamma_1 - \eta_1)^{j_1} (z_1 - \zeta_1)^{k_1} \dots (x_n - \xi_n)^{l_n} (\gamma_n - \eta_n)^{j_n} (z_n - \zeta_n)^{k_n}}{l_1! \dots l_n! j_1! \dots j_n! k_1! \dots k_n!} x \quad (31a)$$

$$x \left\{ \frac{\partial^{\ell}}{\partial x_1^{l_1} \partial y_1^{j_1} \partial z_1^{k_1} \dots \partial x_n^{l_n} \partial y_n^{j_n} \partial z_n^{k_n}} f(\underline{r}_1, \dots, \underline{r}_n) \right\} \begin{matrix} x_i = \xi_i \\ y_j = \eta_j \\ z_k = \zeta_k \end{matrix} \quad (31a)$$

with $l_1 + l_2 + \dots + l_n + j_1 + \dots + j_n + k_1 + \dots + k_n = \ell$

$$\begin{aligned}
 Af = & \frac{1}{n!} \sum_{\substack{l_1, \dots, l_n \\ j_1, \dots, j_n \\ k_1, \dots, k_n}}^{\infty} \frac{1}{l_1! \dots l_n! j_1! \dots j_n! k_1! \dots k_n!} \times \\
 & \times \begin{vmatrix} (x_1 - \xi_1)^{l_1} (\gamma_1 - \eta_1)^{j_1} (z_1 - \zeta_1)^{k_1} & (x_1 - \xi_2)^{l_2} (\gamma_1 - \eta_2)^{j_2} (z_1 - \zeta_2)^{k_2} & \dots & (x_1 - \xi_n)^{l_n} (\gamma_1 - \eta_n)^{j_n} (z_1 - \zeta_n)^{k_n} \\ (x_2 - \xi_1)^{l_1} (\gamma_2 - \eta_1)^{j_1} (z_2 - \zeta_1)^{k_1} & (x_2 - \xi_2)^{l_2} (\gamma_2 - \eta_2)^{j_2} (z_2 - \zeta_2)^{k_2} & \dots & (x_2 - \xi_n)^{l_n} (\gamma_2 - \eta_n)^{j_n} (z_2 - \zeta_n)^{k_n} \\ \vdots & \vdots & \ddots & \vdots \\ (x_n - \xi_1)^{l_1} (\gamma_n - \eta_1)^{j_1} (z_n - \zeta_1)^{k_1} & (x_n - \xi_2)^{l_2} (\gamma_n - \eta_2)^{j_2} (z_n - \zeta_2)^{k_2} & \dots & (x_n - \xi_n)^{l_n} (\gamma_n - \eta_n)^{j_n} (z_n - \zeta_n)^{k_n} \end{vmatrix} \times \\
 (32a) \quad & \times \left\{ \begin{vmatrix} \frac{\partial^{m_1}}{\partial x_1^{l_1} \partial \gamma_1^{j_1} \partial z_1^{k_1}} & \frac{\partial^{m_2}}{\partial x_1^{l_2} \partial \gamma_1^{j_2} \partial z_1^{k_2}} & \dots & \frac{\partial^{m_n}}{\partial x_1^{l_n} \partial \gamma_1^{j_n} \partial z_1^{k_n}} \\ \frac{\partial^{m_1}}{\partial x_2^{l_1} \partial \gamma_2^{j_1} \partial z_2^{k_1}} & \frac{\partial^{m_2}}{\partial x_2^{l_2} \partial \gamma_2^{j_2} \partial z_2^{k_2}} & \dots & \frac{\partial^{m_n}}{\partial x_2^{l_n} \partial \gamma_2^{j_n} \partial z_2^{k_n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^{m_1}}{\partial x_n^{l_1} \partial \gamma_n^{j_1} \partial z_n^{k_1}} & \frac{\partial^{m_2}}{\partial x_n^{l_2} \partial \gamma_n^{j_2} \partial z_n^{k_2}} & \dots & \frac{\partial^{m_n}}{\partial x_n^{l_n} \partial \gamma_n^{j_n} \partial z_n^{k_n}} \end{vmatrix} f(x_1, \dots, x_n) \right\} \\
 & \begin{matrix} x_i = \xi_i \\ \gamma_j = \eta_j \\ z_k = \zeta_k \end{matrix}
 \end{aligned}$$

with $m_\alpha = l_\alpha + j_\alpha + k_\alpha \quad (\alpha = 1, 2, \dots, n)$

Here we find again that $m_1 + m_2 + \dots + m_n \geq N$ where N is a number depending on the number of particles n and their distribution in the four spin and i -spin states. Thus for O^{16} , for example, $N = 2$, for C_{α}^{40} $N = 3$ and so on. In order to include spin and i -spin, we make the assumption that every column of the first determinant in (32a) corresponds to definite spin and i -spin state.

R E F E R E N C E S

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