UNIVERSITY OF OTTAWA

CLUSTERING IN THE NUCLEUS OF Be^8

by

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

Department of Physics,
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The University of Ottawa,
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1964

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Department of Physics

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To Mona and Jennifer

ABSTRACT

At the present time, the meaning of the cluster model and what is meant by clustering in actual nuclei has not been fully clarified. It is thought that some progress is made here in an understanding of clustering in nuclei. Along with defining the cluster model, the amount of ad hoc involved in the choice of a certain cluster model of a nucleus is given. Also presented here, is a quantitative measure of the amount of clustering occurring in the nucleus. A calculation of this measure of the degree of clustering in the Be^8 nucleus is performed with success. It is demonstrated that Be^8 is slighty ellipsoidal in shape and much less dense than a free alpha particle. The radius of the alpha particles within Be^8 is calculated and compared with the radius of a free alpha particle. The separation of the alpha particles is found to be much less than the magnitude of the alpha cluster radius. This investigation also revealed certain new mathematical and physical properties of the cluster model.

ACKNOWLEDGEMENTS

I wish to acknowledge with gratitude the fact that Dr. R.C. Smith was very helpful through his interest in this work. I am also grateful to Computing Devices of Canada for the generous provision of their computing facilities. This work was partially supported by Grants A823 and A1866 from the National Research Council of Canada.

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CHAPTER 1

INTRODUCTION

A number of nuclear models have been developed to describe the nucleus. The cluster model is a recent one that has had much success in the description of the lower energy levels in light nuclei.

Since it is established that nuclei are composed of neutrons and protons, the cluster model attempts to choose a wave function to describe the behaviour of these nucleons. The choice of this wave function is the basis of the model. The wave function is not obtained as an exact solution of the many-body problem from the knowledge of the elementary nucleon-nucleon interaction. First of all the elementary interaction is still unknown, and even if it were known the mathematical difficulties in solving such a many-body problem would be such that we would have to content ourselves with many mathematical approximations. The choice of this cluster model wave function is at first partially ad hoc. Then, since many properties of the nucleus can be described by an independent particle model (i.e. the simple shell model) the cluster model is "stabilized" into the realm of the simple shell model. This tends to make the cluster model wave function realistic. Although the two models are in general different, it is often possible to make a connection between them, depending upon the particular nucleus in question.

To get a physical picture of a nucleus that can be described by a cluster model is not an easy thing to do. We may have a wave function that describes the nuclear properties very well, but the problem of a physical interpretation is awkward. Although the cluster model may describe a nucleus, how do we know if there is any actual clustering going on in the nucleus? Cluster model wave functions are usually of a form such that the determination of the probability of finding any one nucleon at a given distance from the nuclear center of mass is a formidable one. The position of any one nucleon with respect to the mass center generally depends in some complicated way on the position of each of the other nucleons. If the cluster wave function were some linear combination of individual particle wave functions (not independent particle model wave functions) the problem of interpreting the wave functions would not be difficult. Unfortunately this is not the case.

Tang and Wildermuth* (1) have done a wave function analysis of a cluster model for Li^6 and showed that a limit exists in which there is clustering in the extreme, with two noninterpenetrating clusters. They found that the degree of clustering depends upon the value of the ratio of two "width parameters" arising in the wave function. It is shown that for the limiting values of zero there exists extreme clustering while for the value unity the wave function is an eigenfunction of the independent particle model hamiltonian. They made no attempt to examine the amount of clustering at other values of this width parameter ratio.

In this thesis an analysis of the degree of clustering in Be^8 is carried out. First, a treatment similar to theirs is applied to Be^8. Further work is then done for the purpose of learning more about the

* References will be found in a bibliography at the end of the thesis.

amount of real clustering that occurs in this nucleus. A measure of the degree of clustering in the model for values of the width parameter ratio other than the zero limit is also determined. This measure is obtained by a calculation of the expected relative separation between the clusters, and the value of the r.m.s. radius of the alpha clusters.

CHAPTER 2

THE CLUSTER MODEL

For the purpose of developing certain results that are later employed in this thesis,a general review of the cluster model is presented in this chapter.First,the theory of the independent particle model with a harmonic oscillator potential (the simple shell model)is briefly considered in a light which makes the cluster model seem quite plausible.This is followed by the development of,first,the simple cluster model and then the generalized cluster model.

A historical account of the development of the cluster model is not attempted and the cluster model presented here has been derived mainly from the work of Wildermuth (1) and his coworkers.The description of nuclei by a theory of substructures probably came about mainly through the work of Wheeler (18) .This method of description of nuclei has subsequently been studied by many others.

In the last section of this chapter a problem arises of whether or not the eigenfunctions of the generalized cluster model form a complete set.This is an all important question, for only if a complete set of eigenfunctions exist can the cluster model be considered possible for the complete description of the nucleus.

1. The Independent Particle Model

Consider the independent particle model in which a harmonic oscillator well is assumed for the common potential in which each of the nucleons of some particular nucleus moves. For this potential, the Schoedinger equation for the motion of A nucleons has the following form:

$$\frac{1}{2m}\left(\sum_{i=1}^{A}\vec{p}_i + a^2\hbar^2\sum_{i=1}^{A}\vec{r}_i^{\,2}\right)\psi_\alpha = E_\alpha\psi_\alpha \qquad \ldots(1)$$

where:

m is the mass of each of the nucleons, $\vec{p}_i$ is the momentum operator for the ith nucleon, $\vec{r}_i$ is the position vector of the ith nucleon. E_α is the αth energy eigenvalue, ψ_α is the eigenfunction corresponding to the energy eigenvalue E_α, $a = \frac{m\omega}{\hbar}$ is the "width parameter" of the oscillator potential, ω is the classical frequency of the oscillator potential, and α corresponds to a set of quantum numbers compatible with the overall state of the system.

The value of the width parameter, a, is chosen such that the expected value of $\sqrt{\langle r_i^2 \rangle}$ coincides with the experimental r.m.s. radius of the nucleus being considered.

The eigenfunctions, ψ_α, satisfying the above equation of motion and the normal quantum mechanical boundary conditions, can be written as follows:

$$\psi_\alpha = \prod_{i=1}^{A} A_i \exp\left[-\frac{ar_i^2}{2}\right] r_i^{\ell_i} L_{N_i-1/2}^{\ell_i+1/2}(ar_i^2)\, Y_{\ell_i}^{m_i}(\Omega_i) \qquad \ldots(2)$$

$N_i = 0,1,2,3---$; $\ell_i = 0,1,2,3,---N_i$; $m_i = \ell_i, \ell_i-1, \ell_i-2, --- -(\ell_i-2)-(\ell_i-1),-\ell_i$

When N_i is even ℓ_i is even, and when N_i is odd ℓ_i is odd.

In equation (2),

A_i is the normalization constant*:

$$A_i = \left[\frac{2a^{\frac{3}{2}}\,\Gamma\left(\frac{N_i-\ell_i+1}{2}\right)}{\Gamma\left(\frac{N_i+\ell_i+1}{2}\right)}\right]^{\frac{1}{2}},$$

$L_{\frac{N_i-\ell_i}{2}}^{\ell_i+\frac{1}{2}}(x)$ is the associated Laguerre Polynomial (for a table of values, see reference (4)).

$Y_\ell^m(\Omega)$ is the normalized spherical harmonic function with phases chosen as in Condon and Shortley (ref. no.12), and $\Gamma(q)$ is the gamma function:

$$\Gamma(q+1) = \int_0^\infty x^q e^{-x} dx = q\,\Gamma(q).$$

The eigenfunctions, ψ_α, form a complete set of orthogonal wave functions. It is seen that ψ_α is a product of the single particle eigenfunctions. Introducing the intrinsic and isotopic spin coordinates, the single particle

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* See Appendix 1.

eigenfunctions corresponding to the ith particle become:

$$\psi_{p_{\alpha_k}^{i}} = A_i \exp\left[-\frac{ar_i^2}{2}\right] r_i^{\ell_i} L^{\ell_i+1}_{\frac{N_i-\ell_i}{2}} (ar_i^2)\, Y^{m_i}_{\ell_i} (\Omega_i)\, x\, (s_i, t_i) \qquad \ldots(3)$$

where

$\psi_{p_{\alpha_k}^{i}}$ is a particular single particle eigenfunction describing the i'th particle, x is a charge-spin function, s_i is the intrinsic spin quantum number of particle "i", introduced here as a coordinate, t_i is the isotopic spin quantum number of particle "i", introduced here as a coordinate, and $p_{\alpha_k}^{i}$ is a set of single particle quantum numbers, (N_i, ℓ_i, m_i), describing the quantum state of particle "i" compatible with the overall particular state of the system. The subscript "k" denotes the k'th set from all the possible sets.

So far, the Pauli exclusion principle has not been incorporated into the independent particle model wave function, given by equation 3. This will be done after a consideration of the effect of the indistinguisability of the nucleons in a quantum mechanical system.

2. Indistinguishability of Nucleons in Nuclei

When the intrinsic and isotopic spin quantum numbers, s_i and t_i, are treated as coordinates of the system, we may treat the nuclear system of protons and neutrons as a system of indistinguishable particles. Classically it is possible, in principle, to distinguish between the different particles of a system even though they are identical. That is, we could label them at some instant and observe their motion without disturbing the system, and be able to say which is particle 1 and particle 2 (for example) at any time later. In a quantum mechanical description this is not possible because the uncertainty principle does not allow one to observe the motion of the particles constantly without changing the behaviour of the system. Also the overlapping of the wave function associated with each of the identical particles would make it impossible to tell which wave function was associated with which identical particle. A correctly formulated quantum theory of such systems must therefore take explicit account of the indistinguishability of identical particles.

Since the identical nucleons are indistinguishable any physically measureable quantity must be independent of the assignment of the labels. It turns out (see, for example, reference 5) that the only total wave functions which satisfy this requirement on the system are wave functions that are either symmetric or antisymmetric with respect to an interchange of any two particles. Functions of mixed symmetry do not satisfy this condition. (The Pauli principle can be satisfied only if the total wave function is antisymmetric, so the possibility of symmetric wave functions is rejected).

This lack of dependence of physically measureable quantities upon the labeling of the system associated with the antisymmetrized total wave function gives the reason why the expected relative separation of the clusters will serve as a measure of the amount of clustering, even though different particles would be in different clusters at different times. If the particles were distinguishable and the above property were not required, then, even though there may be real clustering* in a system, the average relative separation may be zero and would be approximately zero. This follows from the fact that the different distinguishable particles are equally likely to be in each cluster at different times, which in turn follows from the symmetry of the system. So then, the possibility of obtaining a measure of the degree of clustering through the expectation value of the relative separation of the clusters results from the quantum mechanical nature of the nuclear system. Finally it is noteworthy that due to the indistinguishability of the nucleons it is both necessary and sufficient that the average relative cluster separation be approximately zero if there exists no clustering. However if the particles were distinguishable, there may be no clustering and yet the value of the average cluster separation is quite different from zero and also the average separation could be of approximately zero magnitude while real clustering exists.

* The phrase "real clustering", means (for the case of Be^8) that the nucleus has the shape of a dumbbell. A greater degree of real clustering is associated with a more "dumbbelled" shape of the nucleus.

3. Incorporation of the Exclusion Principle in the Independent Particle Model

The incorporation of the Pauli principle in the overall nuclear system of indistinguishable nucleons requires that the wave function be antisymmetric with respect to an interchange of any two particles. The wave function of the system in a particular state "p" is therefore given by:

$$\psi_{(p_{\alpha_m}^{1} -- p_{\alpha_k}^{i} --- p_{\alpha_n}^{A})} = \mathcal{A} \prod_{i=1}^{A} \psi_{p_{\alpha}^{i}} \qquad \ldots(4)$$

where

$\mathcal{A}$ is an antisymmetrization operator, and $(p_{\alpha_m}^{1} --- p_{\alpha_k}^{i} -- p_{\alpha_n}^{A})$ is a possible set of single particle sets of quantum numbers compatible with the overall state "p" of the system.

The notation is such that $p_{\alpha_k}^{i}$ and $p_{\alpha_k}^{j}$ both denote the k'th set of single particle quantum numbers, in the first case however the symbol i implies that particle 'i' has the k'th set while in the second case particle "j" has this k'th set of quantum numbers. The antisymmetrization can be accomplished by writing the total wave function as a determinant:

$$\psi_{(p_{\alpha_m}^{1} -- p_{\alpha_j}^{A})} = \psi_p = \frac{1}{\sqrt{A!}} \begin{vmatrix} \psi_{p_{\alpha_1}^{1}} & \psi_{p_{\alpha_2}^{1}} & ----- & \psi_{p_{\alpha_A}^{1}} \\ \psi_{p_{\alpha_1}^{2}} & \psi_{p_{\alpha_2}^{2}} & ----- & \psi_{p_{\alpha_A}^{2}} \\ ---- & ---- & ---- & ---- \\ \psi_{p_{\alpha_1}^{A}} & \psi_{p_{\alpha_2}^{A}} & ----- & \psi_{p_{\alpha_A}^{A}} \end{vmatrix} \qquad \ldots(5)$$

The rows refer to the particles and the columns to the single particle quantum states. The general wave function, considering all the possible overall states of the system, is then of the following form:

$$\Psi = \sum_{p=1}^{\infty} a_p \psi_p \qquad \ldots(6)$$

The eigenfunctions of the system of independent nucleons, ψ_p, form at least a physically complete set.* It is seen from the determinant expression for ψ_p that:

$$\int \psi_p^* \psi_q \, d\tau = \delta_{pq} \qquad \ldots(7)$$

where "p" and "q" correspond to two different overall states of the system. δ_{pq} is the Krönecker delta and $d\tau$ is the elemental volume involving all 5A coordinates. Also it is clear that $\left| a_p \right|^2$ is the probability of finding the overall system in the particular state "p". This complete set of orthogonal wave functions will henceforth be referred to as the independent particle wave function system, and the corresponding model the independent particle or simple shell model.

4. Separation of the Independent Particle Equation of Motion by a Cluster System of Coordinates

The previous method of separation of the Schroedinger equation for independent particles is not unique. Another method will now be employed.

Just as one finds that certain problems in physics can be treated more simply in a certain coordinate system, one hopes that a different separation of equation (1) will provide a system of eigenfunctions which describe a real nucleus in a simpler manner than the independent particle eigenfunctions. Perhaps an actual nucleus can be described by a linear superposition of the eigenfunctions involving fewer terms than in the system of coordinates just considered.

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* By physical completeness it is meant, here, that:

$$\lim_{n \to \infty} \int \left(F - \sum_{p=1}^{n} a_p \psi_p\right)^2 d\tau = 0$$

where F is any function satisfying the same boundary conditions as ψ_p.

We now divide the A nucleons into "k" clusters with the number of nucleons in each cluster denoted by $n_1, n_2, ----n_k$. It follows that:

$$\sum_{i=1}^{k} n_i = A$$

The center of mass coordinate of the i'th cluster is given by:

$$R_i = \frac{1}{n_i} \sum_{q=1}^{n_i} \vec{r}^{\,i}_q$$

where

$\vec{r}^{\,i}_q$ is the position vector of the q'th nucleon in the i'th cluster.

The relative coordinates interior to the i'th cluster are given by:

$$\begin{aligned} \vec{\gamma}^{\,i}_1 &= \vec{r}^{\,i}_1 - \vec{R}_i \\ &\text{-----------} \\ \vec{\gamma}^{\,i}_{n_i} &= \vec{r}^{\,i}_{n_i} - \vec{R}_i \end{aligned} \qquad \ldots(8)$$

In this system of coordinates (henceforth referred to as the cluster coordinate system) the classical hamiltonian, H, becomes (see Appendix 2):

$$H = \frac{m}{2} \sum_{j=1}^{A} \dot{\vec{r}}_i^{\,2} + \frac{a^2\hbar^2}{2m} \sum_{j=1}^{A} \vec{r}_i^{\,2}$$

$$= \frac{m}{2} \sum_{j=1}^{k} \left[\sum_{q=1}^{n_j-1} \dot{\vec{\gamma}}^{\,j\,2}_q + \left(\sum_{q=1}^{n_j-1} \dot{\vec{\gamma}}^{\,j} \right)^2 \right] + \frac{a^2\hbar^2}{2} \sum_{j=1}^{k} \left[\sum_{q=1}^{n_j-1} \vec{\gamma}^{\,j\,2}_q + \left(\sum_{q=1}^{n_j-1} \vec{\gamma}^{\,j}_q \right)^2 \right]$$

$$+ \frac{m}{2} \sum_{j=1}^{k} n_j \dot{\vec{R}}_j^{\,2} + \frac{a^2\hbar^2}{2m} \sum_{j=1}^{k} n_j \vec{R}_j^{\,2}$$

The Schroedinger equation, (1) becomes:

$$\left\{ \sum_{i=1}^{k} H_i + \sum_{i=1}^{k} \frac{P_i^2}{2n_i m} + \sum_{i=1}^{k} \frac{a^2\hbar^2}{2m} n_i R_i^2 \right\} \psi = E\psi \qquad \ldots(9)$$

where

$\vec{P}_i$ is the momentum of the i'th cluster and H_i is a Hamiltonian depending only on the relative coordinates and relative momenta of the nucleons in the i'th cluster.

It is therefore seen that we have a complete set of eigenfunctions for equation (9) with the following form

$$\psi_q = \mathcal{A}\left[\sum_{i=1}^{k} \psi \underset{\text{of the i'th cluster}}{(\text{internal coordinates})} \psi(\vec{R}_i) \right] \qquad \ldots(10)$$

where ψ_q is an eigenfunction describing a state of the nucleons in the cluster coordinates.

By introducing the intrinsic and isotopic spin, the cluster eigenfunctions, ψ_q represent a complete set of wave functions that are antisymmetric with respect to exchange of any pair of coordinates $\vec{r}_1, \vec{r}_2, --- \vec{r}_A$ and the intrinsic and isotopic spin coordinates associated with any two nucleons. In the cluster system of coordinates, the general wave function is written:

$$\Psi = \sum_{q=1}^{\infty} b_q \psi_q \qquad \ldots(11)$$

It should be noted that the eigenfunctions in this cluster system are not, in general, orthogonal to each other as they are in the independent particle wave function system. This is only a mathematical difficulty. It is also seen from the preceding work that an eigenfunction

ψ_p in the independent particle wave function system is not, in general, the same as any one of the eigenfunctions, ψ_q, in the cluster wave function system. However, both are eigenfunctions of the Hamiltonian of the independent particle model. The eigenfunctions of each system form a complete set and therefore either system of functions can describe a real nucleus.

The basis of the simplest form of cluster model is the choice of a particular eigenfunction, ψ_q, in this cluster wave function system with the hope that this single wave function may describe the nucleus. A particular eigenfunction, ψ_q, in the cluster wave function system can be described by a linear superposition of eigenfunctions, ψ_p, from the independent particle wave function system and vice versa. This is possible because of the completeness property of both systems. In general, a linear combination involving more than one eigenfunction from the independent particle wave function system is required to obtain a wave function equivalent to a cluster eigenfunction. From this alone it is apparent that the simple cluster model and the simple shell model are not equivalent.

If a real nucleus can be described by this simple cluster model eigenfunction then we say that there is clustering in its simplest form in this nucleus. This means that one of the coefficients, b_q, used in the description of the nucleus in the cluster wave function system satisfies the condition:

$$\left| b_q \right|^2 \simeq 1$$

and all other b_r are very small.

At first sight, one might think that "clustering in the simplest form" does not necessarily mean that there is any actual clustering in the model at all. It is shown in this thesis that, for Be^8, this intuitive notion is correct and "simple clustering" represents no real clustering.

5. Simple Cluster Model for Be^8

Be^8 is composed of four protons and four neutrons. Since alpha particles are known to be tightly bound, a coordinate system is chosen such that there are two clusters with $n_1 = 4$ and $n_2 = 4$. It follows that

$$\sum_{j=1}^{2} n_j = 8$$

The center of mass coordinates of the clusters are given by

$$R_1 = \frac{1}{4} \sum_{i=1}^{4} \vec{r}_i \qquad \text{and} \qquad \vec{R}_2 = \frac{1}{4} \sum_{i=5}^{8} \vec{r}_i$$

It follows from equation (9) that the classical independent particle model Hamiltonian becomes:

$$H = \sum_{j=1}^{2} \left[\frac{P_j^{\,2}}{2M_i} + \frac{n_j^{\,2} a^2 \hbar^2}{2M_j} R_j^{\,2} + \sum_{i=1}^{3} \frac{m}{2} \dot{\vec{\gamma}}_i^{\,j\,2} + \frac{m}{2} \left(\sum_{i=1}^{3} \dot{\vec{\gamma}}_i^{\,j} \right)^2 + \frac{a^2 \hbar^2}{2m} \sum_{i=1}^{3} \vec{\gamma}_i^{\,j\,2} + \frac{a^2 \hbar^2}{2m} \left(\sum_{i=1}^{3} \vec{\gamma}_i^{\,j} \right)^2 \right] \qquad \ldots (12)$$

or

$$H = H_{cm}^1 + H_{cm}^2 + H_{in}$$

where $M_1 = M_2 = 4m$, $n_1 = n_2 = n = 4$,

H^i_{cm} is the Hamiltonian of the center of mass of the i'th cluster, and

H_{in} is the Hamiltonian depending only upon the internal coordinates of the clusters.

Equation (12) can also be written as follows(see Appendix 3).

$$H = \frac{\vec{P}^2_{cm}}{2M} + \frac{4n^2 a^2 \hbar^2}{2M} \vec{R}^2_{cm} + \frac{P^2_{rel}}{2\mu} + \frac{1}{4} \frac{n^2 a^2 \hbar^2}{2\mu} \vec{R}^2_{rel} + \sum_{j=1}^{2} \left[\frac{m}{2} \sum_{i=1}^{3} \dot{\vec{\beta}}^{j\,2}_i + \frac{a^2 \hbar^2}{2m} \sum_{i=1}^{3} \vec{\beta}^{j\,2}_i \right] \qquad \ldots(13)$$

where

$$M = \sum_{i=1}^{8} m_i = 8m;$$

$$\mu = \frac{M_1 M_2}{M_1 + M_2} = 2m; \quad \vec{R}_{cm} = \frac{\vec{R}_1 + \vec{R}_2}{2}; \quad \vec{R}_{rel} = \vec{R}_1 - \vec{R}_2;$$

$\vec{P}_{cm} = M \dot{\vec{R}}_{cm}$ is the classical momentum of the center of mass which is canonically conjugate to $\vec{R}_{cm}$ and $\vec{P}_{rel} = \mu \dot{\vec{R}}_{rel}$ is the classical momentum vector in the relative coordinates which is canonically conjugate to $\vec{R}_{rel}$.

Also $\vec{\beta}^j_1 = \vec{\gamma}^j_2 + \vec{\gamma}^j_3$: $\vec{\beta}^j_2 = \vec{\gamma}^j_3 + \vec{\gamma}^j_1$; $\vec{\beta}^j_3 = \vec{\gamma}^j_1 + \vec{\gamma}^j_2$.

The classical momentum in the $\vec{\beta}$ coordinates is obviously $\vec{p}_\beta \; m\dot{\vec{\beta}}_i$ and is canonically conjugate to $\vec{\beta}_i$. Of course, for our considerations the classical momentum is replaced by its operator form, $P_{cm} = \frac{\hbar}{i} \vec{\nabla}_{cm}$ etc.

The Schroedinger equation for eight independent particles in a harmonic oscillator well transformed into the cluster coordinate system therefore separates as follows:

$$\begin{aligned}
&\left[\frac{\vec{P}_{cm}^{\,2}}{2M} + \frac{4n^2a^2\hbar^2}{2M}\,\vec{R}_{cm}^{\,2}\right]\psi_{cm} = E_{cm}\,\psi_{cm} \\
&\left[\frac{\vec{P}^{2}_{rel}}{2\mu} + \frac{1}{4}\,\frac{n^2a^2\hbar^2}{2\mu}\,\vec{R}^{2}_{rel}\right]\psi_{rel} = E_{rel}\,\psi_{rel} \\
&\left\{\sum_{i=1}^{3}\left[\frac{\vec{p}_{\beta}^{\,1^{2}}}{2m} + \frac{a^2\hbar^2}{2m}\,\vec{\beta}_{i}^{\,1^{2}}\right]\right\}\psi^{1} = E^{1}_{in}\,\psi^{1} \qquad \ldots(14) \\
&\left\{\sum_{i=1}^{3}\left[\frac{\vec{p}_{\beta}^{\,2^{2}}}{2m} + \frac{a^2\hbar^2}{2m}\,\vec{\beta}_{i}^{\,2^{2}}\right]\right\}\psi^{2} = E^{2}_{in}\,\psi^{2}
\end{aligned}$$

where: ψ^1 is the wave function associated with the internal coordinates of cluster "1" and is a function of the independent coordinates $\vec{\beta}^1_1$, $\vec{\beta}^1_2$, $\vec{\beta}^1_3$, ψ^2 is the wave function connected with cluster "2" in the same way that ψ^1 is connected with cluster "1", E^1_{in} is the eigenvalue of the energy to cluster "1" and is associated with ψ^1, E^2_{in} is the eigenvalue of the energy internal to cluster "2" and is associated with ψ^2, E_{cm} is the eigenvalue of the energy of the center of mass of the nucleus (the center of mass motion is eventually discarded), E_{rel} is the eigenvalue of the energy of relative motion of the mass centers of the two clusters, ψ_{cm} is the eigenfunction associated with E_{cm}, and ψ_{rel} is the eigenfunction associated with E_{rel}. Only under certain circumstances is this wave function sufficient to describe the relative motion of the two clusters. This will be shown rigourously in Chapter 3. p_β is the momentum operator that is canonically conjugate to $\vec{\beta}_i$.

Comparing the form of the preceding equations with the three dimensional harmonic oscillator differential equation

$$\left[\frac{\vec{p}^{\,2}}{2m} + \frac{a^2\hbar^2}{2m}\,\vec{r}^{\,2}\right]\psi = E\psi$$

where, $\vec{p} = \frac{\hbar}{i}\vec{\nabla}$ and $E = (N + \frac{3}{2})\,\hbar\omega = (N + \frac{3}{2})\,\frac{\hbar^2 a}{m}$,

it follows that:

$$E_{rel} = (N + \frac{3}{2})\,\frac{\hbar^2 na}{2\mu} = (N + \frac{3}{2})\,\frac{\hbar^2 a}{m}$$

$$E_{cm} = (N' + \frac{3}{2})\,\frac{\hbar^2 2na}{M} = (N' + \frac{3}{2})\,\frac{\hbar^2 a}{m} \qquad \ldots(15)$$

$$E^1_{in} = (N'' + \frac{3}{2})\,\frac{\hbar^2 a}{m}$$

$$E^2_{in} = (N''' + \frac{3}{2})\,\frac{\hbar^2 a}{m}$$

where N, N', N'', and N''' are all positive integers.

From the separated equations of motion it follows that an eigenfunction in this cluster coordinate system has the general form:

$$\psi_q = \mathcal{A}\left\{\psi_k(\alpha_1)\,\psi_m(\alpha_2)\,\psi_{rel}\,\psi_{cm}\,\chi(s_1, t_1, --, s_8, t_8)\right\} \qquad \ldots(16)$$

$\psi_k(\alpha_1)$ is a function that depends on the nine independent internal coordinates of the first alpha cluster and $\psi_m(\alpha_2)$ depends on the nine independent internal coordinates of the second cluster. The subscripts "k" and "m" denote sets of quantum numbers that give the quantum states of $\psi_k(\alpha_1)$ and $\psi_m(\alpha_2)$ respectively. The operator $\mathcal{A}$ denotes the complete antisymmetrization of the wave function with respect to an interchange of any two particles, whose coordinates include the intrinsic and isotopic spin coordinates. X represents a charge-spin function depending upon the intrinsic and isotopic spin coordinates. From the form of the separated equations of motion it is seen that, except for the charge-spin function all the constituent functions composing ψ_q are oscillator wave functions.

The present object is to use the cluster model to describe the ground state and low-lying excited states of Be^8. In order to do this, a more detailed specification of the cluster model is required. For a further specification of the model one must say something more about the constituents of ψ_q given in equation (16). Now, it was pointed out on page 14 that alpha particles are tightly bound. This fact leads to the supposition that the internal states of the two clusters are those corresponding to the lowest energy eigenvalues. Eventually the effect of the center of mass motion will be discarded, but for the moment, to keep in the realm of the simple shell model, we shall keep it and choose the lowest state of the center of mass motion. (The simple shell model does not account for the superfluous states and three extra degrees of freedom arising from the incorrect treatment of a fixed potential well. For a study of the effects of the fixed potential well on the shell model see reference (7)).

It follows from equation (16) and the preceding enumeration of the particulars that:

$$\psi_q = \mathcal{A}\left\{\psi_o(\alpha_1)\,\psi_o(\alpha_2)\,\psi_{o_{cm}}(R_{cm})\,\psi_{\omega_{rel}}\,X(s_1,\text{--},t_A)\right\} \quad \ldots(17)$$

where $\psi_o(\alpha_1)$, $\psi_o(\alpha_2)$ and $\psi_{o_{cm}}$ are the ground state wave functions representing the first alpha cluster, the second alpha cluster, and the center of mass motion. The symbol ω denotes the set of quantum numbers specifying the state of the relative motion.

The above wave function, ψ_q, is the wave function for the simple cluster model of Be^8 in its low-lying states. So far this ψ_q in the cluster wave function system is an eigen function of the independent particle model Hamiltonian. However, it is clear that the cluster and independent particle model are not the same.

There now remains the problem of choosing the set of quantum numbers, $\omega = (N, \ell, m)$, describing the state of the relative motion for the ground state of Be^8 in this simple cluster model. In establishing this set of quantum numbers the simple cluster model is "stabilized" into the realm of the independent particle model through further incorporation of the Pauli Principle. This is done as follows: for the ground state of Be^8 in the simple shell model there are four nucleons in the "S" state and four in the "P" state. This is a result of the Pauli principle at work in this model. The energy in the ground state of the simple shell model is therefore given by

$$4 \times \frac{3}{2}\hbar\omega + 4 \times \frac{5}{2}\hbar\omega = 16\ h\omega$$

Now, the energy eigenvalues corresponding to $\psi_o(\alpha_1)$, $\psi_o(\alpha_2)$, and $\psi_{o_{cm}}$

are $3 \times \frac{3}{2}\hbar\omega$, $3 \times \frac{3}{2}\hbar\omega$, and $\frac{3}{2}\hbar\omega$ respectively. Therefore, if the ground state energy is the same for the two models, the following condition must be satisfied:

$$16\,\hbar\omega = (N + \frac{3}{2})\hbar\omega + (9 + \frac{3}{2})\hbar\omega\,;$$

the result of this is that N must equal 4 in the ground state. The "simple form" of cluster model has now been completely defined for the ground state. The value of N is also taken to be 4 in the first two excited states.

6. Explicit Simple Cluster Model Wave Function for Be^8.

The cluster model wave function will now be written out explicitly from the solutions of the separated equations of motion in the cluster coordinate system. It is seen from equation (14) that:

$$\psi(\alpha_1) = \sum_{i=1}^{3} \psi^1_{\omega_i}$$

where $\omega_i = (n_i, \ell_i, m_i)$ and

$$\psi^1_{n_i \ell_i m_i} = A_{N_i \ell_i} \exp\left[-\frac{a}{2}\beta_i^2 \right] \beta_i^{\ell_i}\, L_{\frac{N_i - \ell_i}{2}}^{\ell_i + \frac{1}{2}} (\alpha\beta_i^2)\; Y_{\ell_i}^{m_i}$$

But, $n_i = \ell_i = m_i = 0$ for $i = 1,2,3$ in the ground state and the first two excited states. It then follows that

$$\psi^1_{000} = A_{00} \exp\left[-\frac{a\beta_i^2}{2} \right] L_0^{\frac{1}{2}} (a\beta_i^2)\; Y_0^0 = \left[\frac{a}{\pi} \right]^{\frac{3}{4}} \exp\left[-\frac{a\beta_i^2}{2} \right]$$

and $$\psi_o(\alpha_1)\,\psi_o(\alpha_2) = \left[\frac{a}{\pi}\right]^{\frac{9}{2}} \exp\left[-\frac{a}{2}\sum_{i=1}^{6}\beta_i^2\right]$$

Also it is seen from equation (14) that

$$\psi_{N\ell m_{cm}} = K_{N\ell} \exp\left[-\frac{8a}{2}R_{cm}^2\right] R_{cm}^{\ell}\, L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}}\, Y_{\ell}^{m}(\Omega_{cm})$$

where

$$K_{N\ell} = \left[\frac{2(8a)^{\frac{5}{2}} \cdot \Gamma\left(\frac{N-\ell}{2}+1\right)}{\Gamma\left(\frac{N+\ell}{2}\right)+\frac{3}{2}}\right]^{\frac{1}{2}}$$

and

$$\psi_{o_{cm}} = \left[\frac{8a}{\pi}\right]^{\frac{1}{2}} \exp\left[-\frac{8aR_{cm}^2}{2}\right]$$

From equation (14) it is also seen that:

$$\psi_{N\ell m_{rel}} = C_{N\ell} \exp\left[-\frac{2aR^2}{2}\right] R^{\ell}\, L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}}(2aR^2)\, Y_{\ell}^{m}(\Omega) \quad \text{---(18)}$$

where $\vec{R} = \vec{R}_{rel}$ and

$$C_{N\ell} = \left[\frac{2(2a)^{\frac{5}{2}} \cdot \Gamma\left(\frac{N-\ell}{2}+1\right)}{\Gamma\left(\frac{N+\ell}{2}+\frac{3}{2}\right)}\right]^{\frac{1}{2}}$$

The low lying states of Be^8 are therefore described in the cluster model by the following wave function:

$$\psi_q = A\left\{\left(\frac{a}{\pi}\right)^{\frac{9}{2}} \exp\left[-\frac{a}{2}\sum_{i=1}^{6}\beta_i^2\right]\left[\frac{8a}{\pi}\right]^{\frac{1}{2}} \exp\left[-\frac{8aR_{cm}^2}{2}\right] C_{N\ell} \exp\left[-\frac{2aR^2}{2}\right]\right.$$

$$\left. R^{\ell} L^{\ell+\frac{1}{2}}_{\frac{N-\ell}{2}} (2aR^2)\; Y_{\ell}^{m}(\Omega)\; X\right\}$$

where N = 4 for these states. Also it is required that if N is even ℓ must be even. It is known experimentally (Reference 8) that the ground state of Be^8 has a total angular momentum quantum number, "J", equal to zero and is an even parity state. Assuming the ℓ-S coupling scheme, it is seen that $\ell = 0$ is consistent with experiment and also with the simple shell model, when the spin function is given by

$$X(S,T) = \delta(s_1,\tfrac{1}{2})\,\delta(t_1,\tfrac{1}{2})\,\delta(s_2,\tfrac{1}{2})\,\delta(t_2,-\tfrac{1}{2})\,\delta(s_3,-\tfrac{1}{2})\,\delta(t_3,\tfrac{1}{2})\,\delta(s_4,-\tfrac{1}{2})$$

$$\delta(t_4,-\tfrac{1}{2})\,\delta(s_5,\tfrac{1}{2})\,\delta(t_5,\tfrac{1}{2})\,\delta(s_6,\tfrac{1}{2})\,\delta(t_6,-\tfrac{1}{2})\,\delta(s_7,-\tfrac{1}{2})\,\delta(t_7,\tfrac{1}{2})$$

$$\delta(s_8,-\tfrac{1}{2})\,\delta(t_8,-\tfrac{1}{2}) \qquad \ldots(19)$$

where s_i is the intrinsic spin quantum number of the i'th nucleon, t_i is the isotopic spin quantum number of the i'th nucleon, S is the total intrinsic spin quantum number, T is the total isotopic spin quantum number, and both "S" and "T" are zero in these three low lying states.

The simple cluster model wave function for the ground state of Be^8 is given by:

$$\Psi_q = \mathcal{A} \left[\frac{a^{23}\, 2^{15}}{\pi^{23}\, 3^2\, 5^2} \right]^{\frac{1}{4}} \exp\left[-\frac{a}{2} \sum_{i=1}^{6} \beta_i^2 \right] \exp\left[-\frac{8aR_{cm}^2}{2} \right] \exp\left[-\frac{2aR^2}{2} \right]$$

$$L_2^{\frac{1}{2}}(2aR^2)\ \chi(S,T) \qquad \ldots(20)$$

From page 15

$$R_{cm} = \frac{\vec{r}_1+\vec{r}_2+\vec{r}_3+\vec{r}_4+\vec{r}_5+\vec{r}_6+\vec{r}_7+\vec{r}_8}{8}$$

Hence it is seen that $\exp\left[-\frac{8aR_{cm}^2}{2} \right]$ is symmetric with respect to an interchange of any two nucleons. Also $\exp\left[-\frac{a}{2}(\sum_{i=1}^{6} \beta_i^2) + 2aR^2 \right]$ is symmetric with respect to an interchange of any two position vectors, $\vec{r}_i$ and $\vec{r}_j$. For the proof of this, see Appendix 4.

Also

$$L_2^{\frac{1}{2}}(x) = \frac{15}{8} - \frac{5x}{2} + \frac{x^2}{2}$$

Therefore equation (20) can be written as follows:

$$\psi_q = \left[\frac{2^{11}\, a^{23}}{3^2\, 5^2\, \pi^{23}}\right]^{\frac{1}{4}} \exp\left[-\frac{a}{2}\sum_{i=1}^{6}\beta_i^2\right] \exp\left[-\frac{2aR^2}{2}\right] \exp\left[-\frac{8aR_{cm}^2}{2}\right]$$

$$\mathcal{A}\,(4a^2R^4 - 10aR^2 + \frac{15}{4})\,\chi(S,T) \qquad \ldots(21)$$

where $\mathcal{A}$ represents an antisymmetrization operation with respect to an interchange of any two nucleons, including the charge spin and coordinates.

In Appendix 5 it is shown that the antisymmetrization of the function $f(R) = -10aR^2 + \frac{15}{4}$ with respect to the position vector coordinates yields zero. This result is obtained by a further stabilization of the cluster model into the realm of the independent particle model which is partially ad hoc but consistent. This simplifies equation (21).

At this point it is noted that the experimental spin and parity assignment is ($J=0^+$, $T=0$), ($J=2^+$, $T=0$), and ($J=4^+$, $T=0$) in increasing order of the excitation of the states, see reference 8. This assignment also agrees with the simple shell model. Now, in the same way that it was established that $\ell=0$ in the ground state, it can be shown that ℓ is 2 and 4 in the first two excited states. It is now clear that the function

$$R^{\ell}\, L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}}\,(a R^2)$$

is a polynominal of degree N=4, for the ground state and first two excited states of the cluster model. Hence, the unnormalized simple cluster model wave functions for the first three levels of Be^8 is given by

$$\psi_q = \exp\left[-\frac{a}{2}\sum_{i=1}^{6}\beta_i^2\right]\exp\left[-\frac{2aR^2}{2}\right]\exp\left[-\frac{8aR_{cm}^2}{2}\right]\mathcal{A}\left[R^N Y_\ell^m(\Omega)X(S,T)\right] \quad \ldots(22)$$

where N is equal to 4. The effect of the fixed potential well, in the simple shell model, on the center of mass motion can be removed by replacing $\exp\left[-\frac{8aR_{cm}^2}{2}\right]$ by unity.

7. The Generalized Cluster Model

The generalized cluster model will now be defined. It will become clear that the simple cluster model, already discussed, is a special case of this generalized cluster model. Furthermore, it will be seen that the generalized cluster model is a starting point, by the choice of a trial wave function, for the variational method of solution of the many-body Schroedinger equation.

The wave function ψ_q given by equation (22) is an eigenfunction of the original independent particle model Hamiltonian in the cluster wave function system. In the generalized cluster model the width parameter in the exponential term that is dependent upon the relative coordinate R, is replaced by an independent width parameter denoted by "β". Then both width parameters "a" and "β" are allowed to vary. The values of these variational parameters are usually determined by the Ritz variational method in conjunction with the empirical knowledge of the binding energy of an alpha particle. The Ritz variational method utilizes the fact that the minimization of the integral:

$$\lambda = \int \psi^* H \psi \, dv$$

subject to the auxiliary condition

$$\int \psi^* \psi \, dv = 1$$

is exactly equivalent to the problem of solving the Schoedinger equation

$$H \psi = \lambda \psi,$$

where λ corresponds to a Lagrangian multiplier. If the generalized cluster trial wave function had enough variational parameters so that ψ_q could be made to vary in every possible way then the Lagrangian multiplier λ_q would be equal to the true energy eigenvalue λ_q^T of the nucleus. This, of course, assumes the knowledge of a correct nucleon-nucleon interaction; this, in fact, is now known. However, the generalized cluster wave functions have only two variational parameters. The energies of the states obtained in the cluster model, using the correct nucleon-nucleon interaction, are therefore greater than or equal to the true energies of the levels occurring in a nucleus.

The unnormalized generalized cluster wave function for Be^8 in its first three excited states can now be written:

$$\psi_q = \psi_{N\ell m} = \mathcal{A} \exp\left[-\frac{a}{2}\sum_{i=1}^{6} \beta_i^2\right] \exp\left[-\beta R^2\right] \left[R^N Y_\ell^m(\Omega)\, X(S,T)\right] \qquad \ldots(23)$$

where $(N,\ell,m) = (4,0,0)$, $\left(4,2,\begin{smallmatrix}2\\1\\0\\-1\\-2\end{smallmatrix}\right)$, and $\left(4,4,\begin{smallmatrix}4\\3\\2\\1\\0\\-1\\-2\\-3\\-4\end{smallmatrix}\right)$ in the first three states. This is the wave function obtained and used by Wildermuth and Kanellopoulos. (See reference (1) and (13)).

When "β" or "a" or both vary from the value of the width parameter in the closely related simple shell model, the cluster wave function is no longer an eigenfunction of the original simple shell model Hamiltonian given by equation (1). The effective nuclear forces involved in this generalized cluster model are therefore different from those involved in the indépendent particle model. With the introduction of these variational width parameters we no longer have the simple form of cluster model, and it is clear that the generalized cluster wave function now satisfies some differential equation that may not be exactly Schroedingers equation. It is difficult to determine the differential equation whose solutions are the generalized cluster model wave functions. The question "Do the generalized cluster eigenfunctions form a complete set?", now arises. The answer to this remains unknown because we cannot write down the associated differential equation of motion.

CHAPTER 3

PHYSICAL CONTENT OF GENERALIZED CLUSTER WAVE FUNCTIONS FOR Be^8

In this chapter the physical content of the generalized cluster wave function for Be^8 in its ground state and first two excited states will be examined qualitatively. The method of analysis will be similar to that applied to the ground state of Li^6 in reference 3. The correlation, which is useful in later discussions, is first derived.

1. The Correlation Function

Consider the correlation function $D(\vec{r}\,'_1\ {+}{+},\ \vec{r}\,'_2\ {+}{-},\ \vec{r}\,'_3\ {-}{+},\ \vec{r}\,'_4\ {-}{-},\ \vec{r}\,'_5\ {+}{+},\ \vec{r}\,'_6\ {+}{-},\ \vec{r}\,'_7\ {-}{+},\ \vec{r}\,'_8\ {-}{-})$ where $D\ d\vec{r}\,'_1 \mbox{---} d\vec{r}\,'_8$ denotes the probability of finding a nucleon with intrinsic spin quantum number $s_z = \frac{1}{2}$, isotopic spin quantum number $t_z = \frac{1}{2}$ and with a position vector lying between $\vec{r}\,'_1$ and $\vec{r}\,'_1 + d\vec{r}\,'_1$, another nucleon with intrinsic spin $s_z = \frac{1}{2}$, isotopic spin $t_z = -\frac{1}{2}$ lying between $\vec{r}\,'_2$ and $\vec{r}\,'_2 + d\vec{r}\,'_2$, and so on. It is clear that

$$D \alpha \int \Psi^*_{N\ell m} \Big\{ P \Big[\delta(\vec{r}_1 - \vec{r}\,'_1)\, \delta(s_1,\tfrac{1}{2})\, \delta(t_1,\tfrac{1}{2})\, \delta(\vec{r}_2-\vec{r}\,'_2)\, \delta(s_2,\tfrac{1}{2})\, \delta(t_2,-\tfrac{1}{2})$$

$$\delta(\vec{r}_3-\vec{r}\,'_3)\, \delta(s_3,-\tfrac{1}{2})\, \delta(t_3,\tfrac{1}{2})\, \delta(\vec{r}_4-\vec{r}\,'_4)\, \delta(s_4,-\tfrac{1}{2})\, \delta(t_4,-\tfrac{1}{2})\, \delta(\vec{r}_5-\vec{r}\,'_5)$$

$$\delta(s_5,\tfrac{1}{2})\, \delta(t_5,\tfrac{1}{2})\, \delta(\vec{r}_6-\vec{r}\,'_6)\, \delta(s_6,\tfrac{1}{2})\, \delta(t_6,-\tfrac{1}{2})\, \delta(\vec{r}_7-\vec{r}\,'_7)\, \delta(s_7,-\tfrac{1}{2})$$

$$\delta(t_7,\tfrac{1}{2})\, \delta(\vec{r}_8-\vec{r}\,'_8)\, \delta(s_8,-\tfrac{1}{2})\, \delta(t_8,-\tfrac{1}{2}) \Big] \Big\} \Psi_{N\ell m}\ d\tau \qquad \ldots(24)$$

where the integration sign denotes an integration over all 24 spatial coordinates and a summation over the spin and isotopic spin coordinates.

P is the permutation operator on all the nucleon coordinates $\vec{r}$, s and t, and $\Psi_{N\ell m}$ is the generalized cluster model wave function for Be^8 in its ground state and first two excited states.

Since the quantity* $P\left[\delta(r_1-r'_1)\,.\;.\;.\;\delta(t_8,-\frac{1}{2})\right]$ is symmetric in all the coordinates (not a symmetrizing operator) it follows that

$$P\left[---\right]\Psi_{N\ell m} = P\left[---\right]\mathcal{A}\; G_{N\ell m}X(S,T) = \mathcal{A}\,P\left[---\right]G_{N\ell m}X(S,T)$$

where, by definition

$$G_{N\ell m} = \exp\left[-\frac{a}{2}\sum_{i=1}^{6}\beta_i^2\right]\exp\left[-\beta R^2\right]R^N\,Y_\ell^m\,(\Omega)$$

In Appendix 6 it is shown that

$$(\mathcal{A}u)\;(\mathcal{A}v) = \mathcal{S}(u\mathcal{A}v) = \mathcal{S}\,(v\mathcal{A}u)$$

where $\mathcal{S}$ is a symmetrization operator, and u and v are any two functions of the 40 independent variables. This and the fact that $(\mathcal{A}f)^* = \mathcal{A}f^*$, where f is any function, leads to the result

$$\Psi^*_{N\ell m}P\left[---\right]\Psi_{N\ell m} = \mathcal{A}\,(G_{N\ell m}X)^*\,P\left[---\right]\mathcal{A}\,G_{N\ell m}X = \mathcal{A}\,(G_{N\ell m}X)^* \times$$

$$\mathcal{A}\,(P\left[---\right]G_{N\ell m}X) = \mathcal{S}\left\{P\left[---\right]G_{N\ell m}X\mathcal{A}\,(G_{N\ell m}X)^*\right\} = \mathcal{S}\left\{\Psi^*_{N\ell m}P\left[---\right]G_{N\ell m}X\right\}$$

Also, in Appendix 7 it is proved that

$$\int\mathcal{S}f(\vec{x}_1\ldots\vec{x}_N)\;d\tau = \sqrt{N!}\int f(\vec{x}_1\ldots\vec{x}_N)\;d\tau$$

Therefore equation (24) becomes

$$D\alpha\int\Psi^*_{N\ell m}\,P\left[---\right]G_{N\ell m}x(S,T)\;d\tau \qquad \ldots(25)$$

---

* In Appendix 8 $P\left[---\right]$ is replaced by its equivalent form, a permanent, which is defined in Appendix 7.

In Appendix 8 the summation over the intrinsic and isotopic spin coordinates is performed and it is found that

$$D\alpha \int \Big[G^{*}_{N(m} - P_{26} G^{*}_{N\ell m} - P_{15} G^{*}_{N\ell m} - P_{37} G^{*}_{N\ell m} + P_{48} G^{*}_{N\ell m} + P_{48} P_{37} G^{*}_{N\ell m}$$

$$+ P_{37} P_{26} G^{*}_{N\ell m} + P_{48} P_{26} G^{*}_{N\ell m} \Big] G_{N\ell m} (1 + P_{26} + P_{15} + P_{37} + P_{48} + P_{48} P_{37}$$

$$+ P_{37} P_{26} + P_{48} P_{26})$$

$$\delta(\vec{r}_1 - \vec{r}'_1)\ \delta(\vec{r}_2 - \vec{r}'_2)\ \delta(\vec{r}_3 - \vec{r}'_3)\ \delta(\vec{r}_4 - \vec{r}'_4)\ \delta(\vec{r}_5 - \vec{r}'_5)\ \delta(\vec{r}_6 - \vec{r}'_6)\ \delta(\vec{r}_7 - \vec{r}'_7)\ \delta(\vec{r}_8 - \vec{r}'_8)\ d\tau$$

where $P_{ij}\ G_{N\ell m}$ interchanges the spatial coordinates $\vec{r}_i$ and $\vec{r}_j$ in the function $G_{N\ell m}$. If we denote $P_{ij}\ G_{N\ell m}$ by $\psi(ij)$ and $G_{N\ell m}$ by $\psi(o)$ we have, after integrating the correlation function (see Appendix 9);

$$D\alpha \left|\psi(o)\right|^2 + \left|\psi(26)\right|^2 + \left|\psi(15)\right|^2 + \left|\psi(37)\right|^2 + \left|\psi(48)\right|^2 + \left|\psi(48,37)\right|^2 + \Big|$$

$$\psi(37,26)\Big|^2 \quad \left|\psi(48,26)\right|^2 + 2\ \mathrm{Re} \Big[-\psi(o)^{*}\psi(26) - \psi(o)^{*}\psi(15)$$

$$-\psi(o)^{*}\psi(37) - \psi(o)^{*}\psi(48) + \psi(o)^{*}\psi(48,37) + \psi(o)^{*}\psi(37,26)$$

$$+\psi(o)^{*}\psi(48,26) - \psi(15)^{*}\psi(37,48) - \psi(15)^{*}\psi(26,48) - \psi(15)^{*}\psi(15,48)$$

$$+\psi(15)^{*}\psi(37) - \psi(26)^{*}\psi(37,48) - \psi(26)^{*}\psi(26,37) - \psi(26)^{*}\psi(48,26)$$

$$+\psi(26)^{*}\psi(15) + \psi(26)^{*}\psi(37) + \psi(26)^{*}\psi(48) - \psi(37)^{*}\psi(26,37)$$

$$-\psi(37)^{*}\psi(15,37) - \psi(37)^{*}\psi(37,48) + \psi(37)^{*}\psi(48) - \psi(48)^{*}\psi(26,48)$$

$$-\psi(48)^{*}\psi(15,48) - \psi(48)^{*}\psi(37,48) + \psi(48,37)^{*}\psi(26,48) + \psi(48,37)^{*}$$

$$\psi(26,37) + \psi(37,26)^{*}\psi(26,48) + \psi(15)^{*}\psi(48) \Big] \qquad \ldots(26)$$

2. Interpretation of the Correlation Function

Tang, Wildermuth, and Pearlstein (Reference 3) have calculated the corresponding correlation function associated with the cluster model of Li^6. They state that it can be shown that the values of the cross terms appearing in their correlation function approach zero in the limit as the ratio of their two width parameters, $\frac{\beta}{\alpha}$, approaches zero, and that only one of the remaining terms is significant at any one instant of time. It is shown in the next chapter that the consequences of their claim in the determination of clustering are approximately valid for Be^8 in the ground state.

For the moment, it will be assumed that the cross terms do go to zero and that only one of the remaining terms is significant at any one time. The consequences of this assumption will now be studied.

With the preceding assumptions the correlation function becomes

$$D \alpha \ \psi(o)^2 + \psi(26)^2 + \psi(15)^2 + \psi(37)^2 + \psi(48)^2 + \psi(48,37)^2 + \psi(37,26)^2 + \psi(48,26)^2$$

where only one of the terms is significant at any one instant of time. Hence, with this assumption, the probability of finding a nucleon with intrinsic spin $s_z = \frac{1}{2}$, isotopic spin $t_z = \frac{1}{2}$, lying between $\vec{r}'_1$ and $\vec{r}'_1 + d\vec{r}'_1$, another nucleon with intrinsic spin $s_z = \frac{1}{2}$, isotopic spin $t_z = -\frac{1}{2}$, lying between $\vec{r}'_2$ and $\vec{r}'_2 + d\vec{r}'_2$, and so on, is given by one of the terms in the last expression multiplied by $d\vec{r}_1 \ldots d\vec{r}_8$. Each of the terms is of the form of a product of two internal alpha particle wave function intensities multiplied by the relative wave function intensity. Because the effective contribution to the correlation function is always in this form we can write

$$D\alpha \left|\psi(\alpha_1)\right|^2 \left|\psi(\alpha_2)\right|^2 \left|R^N\right| \exp\left[-\beta R^2\right] \left|Y_\ell^m(\Omega)\right|^2$$

After summing over the spin coords the remaining correlation function can also be expressed as follows: It is the probability of finding the eight nucleons arranged such that the independent coordinates, $\vec{\beta}_1$, $\vec{\beta}_2$, $\vec{\beta}_3$, $\vec{\beta}_4$, $\vec{\beta}_5$, $\vec{\beta}_6$, and $\vec{R}$, describing the position of the nucleons have values in the range $\vec{\beta}'_1$ and $\vec{\beta}'_1 + d\vec{\beta}'_1, \ldots, \vec{R}'$ and $d\vec{R}'$. Integrating over all coordinates except "R" one obtains the result that the probability distribution describing the relative separation of the clusters is given by

$$D = \frac{2^{11+\frac{1}{2}}\, \epsilon^{5+\frac{1}{2}}\, (\sqrt{a}\, R')^{10}}{3^3 \times 7 \times 5 \sqrt{\pi}} \exp\left[-2\epsilon\, (\sqrt{a}\, R')^2\right] \qquad \ldots(26a)$$

where $\epsilon = \frac{\beta}{a}$

The above expression gives the probability that the value of $\sqrt{a}\,R$ lies between $\sqrt{a}\,R'$ and $\sqrt{a}\,(R' + dR')$ for small values of ϵ. In the realm of the cluster model, the above result shows that for small values of the quantity ϵ, the nucleons are arranged in a cluster form such that the most probable value of the relative separation of the clusters is given by $R = \sqrt{\frac{5}{2\beta}}$. From Figure 1 it is seen that as ϵ becomes small the distribution curve becomes what would be expected for the case of two independent and distinquishable alpha particles. From this result, it can now be stated that if the assumptions made here concerning the significant terms in the correlation function are valid, then for small values of ϵ there is a large probability for the formation of two distinct and non-interpenetrating alpha particles, and the most probable separation of the clusters is given by $R = \sqrt{\frac{5}{2\beta}}$. In the next chapter the expected value of the separation of clusters is evaluated for all values of ϵ. However it is noted that through the use of the correlation function obtained here, it is possible to obtain the probability distribution of the relative separation of the clusters for all values of the variational parameters α and β. This probability distribution is obtained by integrating the correlation function on page 30 over all coordinates except R. The resultant function multiplied by R^2dR is proportional to the probability of R' lying between R and R+dR.

The quantitative considerations in the next chapter agree with the result that the cluster separation becomes infinitely large as ϵ approaches zero. Furthermore it is discovered that the expected root mean square radius of the alpha cluster approaches infinity as ϵ goes to zero. However it's rate of approaching infinity is less than the rate at which the separation approaches infinity for ϵ going to zero. In fact the ratio of the separation to the radius approaches infinity with ϵ going to zero.

Figure 1

The approximate probability distribution of the normalized separation between the two alpha clusters under the assumption that the cross terms is the correlation function on page 30 are zero and that only one of the remaining terms is significant at any one instant of time.

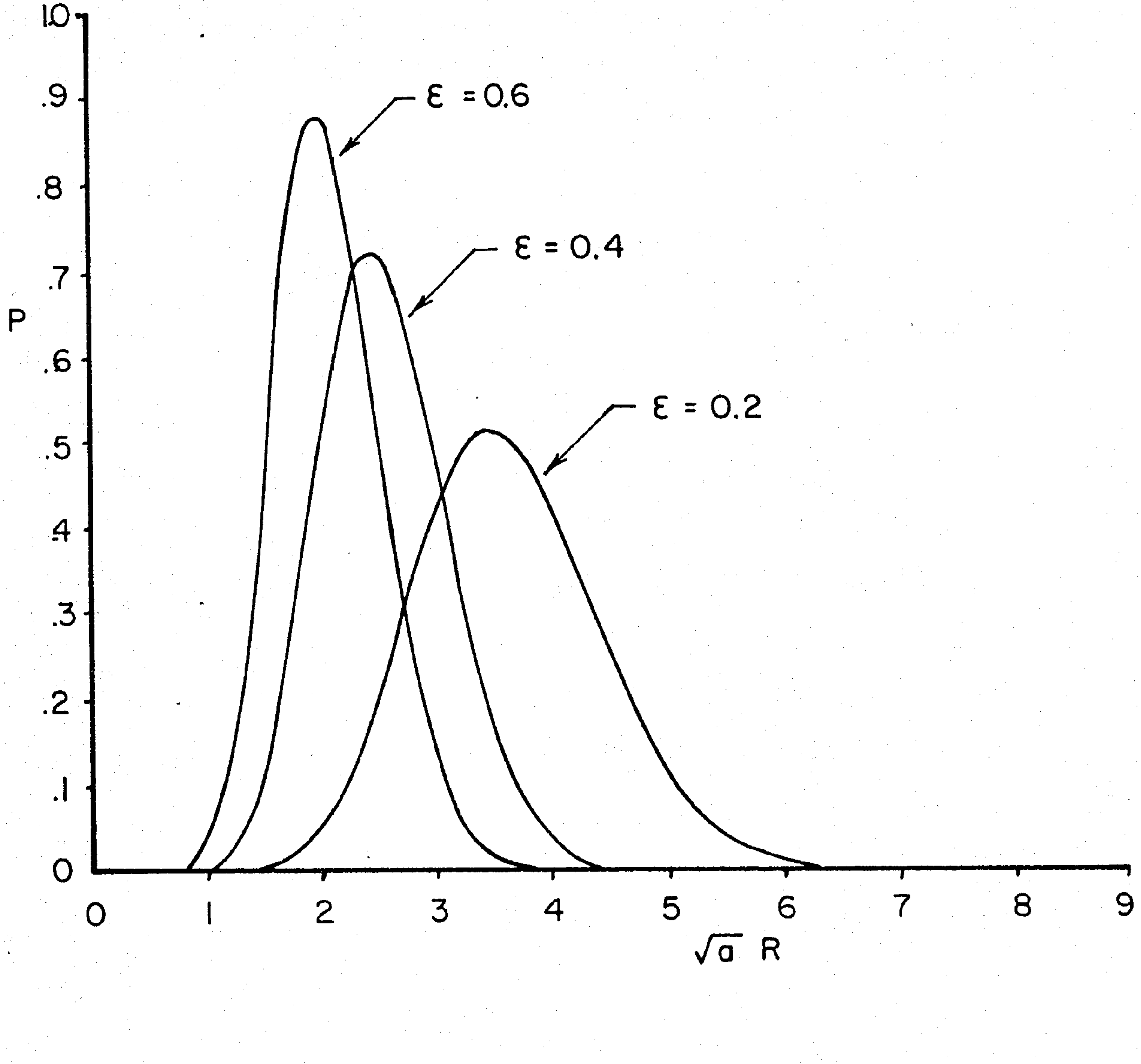
$R = \sqrt{\frac{5}{2\beta}}$ = most probable separation of the clusters

$R = \frac{1.621}{\sqrt{\beta}}$ = average or expectation value of the separation of the clusters

$Pxd(\sqrt{a}R') =$ probability that $\sqrt{a}R$ lies between $\sqrt{a}R'$ and $\sqrt{a}R' + \sqrt{a}dR'$

a = variational parameter in the generalized cluster wave function

R = separation of the clusters


1.0
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
P
ε = 0.6
ε = 0.4
ε = 0.2
0
1
2
3
4
5
6
7
8
9
√a R

3) Chi-Square Analysis with Controls

Following the discriminant analysis, a second chi-square analysis was performed to determine the association between ethnolinguistic status and value hierarchies while controlling for the effects of socio-economic status. In this analysis, subjects were formed into more homogeneous groups based upon this variable and the chi-square was then computed for these groupings of Anglophone versus Francophone.

D. Presentation of Results

a) Description of Subject Pool

Of the 534 subjects tested, a total of 216 students who met the criteria outlined in the methodology (100 Anglophone and 116 Francophone) participated. The students were from eight faculties of the University of Ottawa (see Table II). Eighty (37%) males and 136 (63%) females participated. The subjects were divided by sex into 22.2% Francophone males and 14.8% Anglophone males; 31.0% Francophone females and 32.0% Anglophone females. The mean age of the sample was 23.5 years (s.d. = 6.07) with a range of 42 years (17 to 59 years). The majority of the students (81.9%) were registered as full-time and the mean number of years of completed schooling was 15.17 (s.d. = 1.75). Table III reports the distribution of the sample according to provincial birthplace.

The values of "β" and "a" obtained by Pearlstein, Tang and Wildermuth(2) for the minimized energy eigenvalues are used to get a measure of the actual amount of clustering in the Be^{8} nucleus. Also the root expected square radius of the clusters is evaluated as a function of β and a. Various combinations of these quantities provide useful information about the physical interpretation of the cluster model and also a quantitative measure of the amount of real clustering that exists in the Be^{8} nuclei.

It is demonstrated that to calculate the square root of the expected square of the cluster radius and separation exactly is a formidable task. Fortunately, it becomes clear that a very satisfactory approximation can be made in the antisymmetrization of the cluster model wavefunction. The problem is then reduced to one that can be solved with a finite amount of work.

While investigateing the Be^{8} nucleus from the cluster model view point various mathematical and physical properties of the cluster model were uncovered and are discussed in this chapter. These properties of the cluster model provide a further insight into the model itself and also provide convenient techniques which are useful when nuclear structure problems can be projected into the cluster model

1. Operator Expectation Value Considerations

It is clear that the expectation value of an operator, $\mathcal{O}$, can be written in the following form

$$N^2\langle\mathcal{O}\rangle = \frac{1}{8!}\int d\tau \int G^*_{n\ell m}(\ \ldots\ \vec{r}\,''_i\ \ldots)\, X(S,T)''$$

$$\begin{vmatrix} \delta(\vec{r}_1 - \vec{r}\,''_1)\,\delta(s_1,s''_1)\,\delta(t_1,t''_1) & \ldots & \delta(\vec{r}_1 - \vec{r}\,''_8)\,\delta(s_1,s''_8)\,\delta(t_1,t''_8) \\ \ldots & \ldots & \ldots \\ \delta(\vec{r}_8 - \vec{r}\,''_1)\,\delta(s_8,s''_1)\,\delta(t_8,t''_1) & \ldots & \delta(\vec{r}_8 - \vec{r}\,''_8)\,\delta(s_8,s''_8)\,\delta(t_8,t''_8) \end{vmatrix} d\tau''$$

$$\mathcal{O}\int G_{n\ell m}(.\ \vec{r}\,'_i\ ..)\, X(S,T)' \begin{vmatrix} \delta(\vec{r}_1 - \vec{r}\,'_1)\,\delta(s_1,s'_1)\,\delta(t_1,t'_1) & \ldots & \delta(t_1,t'_8) \\ \ldots & \ldots & \ldots \\ \delta(\vec{r}_8 - \vec{r}\,'_1)\,\delta(s_8,s'_1)\,\delta(t_8,t'_1) & \ldots & \delta(t_8,t'_8) \end{vmatrix} d\tau'$$

where the integrations include a summation over the spin coordinates. N^2 is the square of the normalization constant and is equal to the right hand side of the above equation with $\mathcal{O}=1$. Recalling the expression for the charge-spin function on page 22 it follows that after performing the summation over the spin coordinates this equation becomes so elaborate that one wouldn't consider putting it into print. One is now confronted with the fact that the problem of determining the expectation value of some general operator is unfeasible unless that operator possesses some special property or unless some sensible approximations can be made. For the case of dynamical operators that are invariant with respect to an interchange of any two particles the expected value of the operator can be obtained in a relatively simple way. For reasons either immediately obvious, or soon to become apparent, it is convenient to introduce this invariant operator, $\mathcal{O}$. The quantity that will now be calculated is

$$\langle \mathcal{O} \rangle = \frac{\int \psi^*_{N\ell m}\, \mathcal{O}\, \psi_{N\ell m}\, d\tau}{\int \psi^*_{N\ell m}\, \psi_{N\ell m}\, d\tau} \qquad \ldots(27)$$

where integral signs include a summation over the spin coordinates. In Appendix 11 it is shown that equation 27 can be reduced to the following form

$$N^2 \langle \mathcal{O} \rangle = \iint G_{N\ell m}(\vec{r}\,'_1 \ldots \vec{r}\,'_8)^* X(S', T')^*$$

$$\begin{vmatrix} \delta(\vec{r}_1 - \vec{r}\,'_1)\, \delta(s_1, s'_1)\, \delta(t_1, t'_1) \ldots \delta(\vec{r}_1 - \vec{r}\,'_8)\, \delta(s_1, s'_8)\, \delta(t_1, t'_8) \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \delta(\vec{r}_8 - \vec{r}\,'_1)\, \delta(s_8, s'_1)\, \delta(t_8, t'_1) \ldots \delta(\vec{r}_8 - \vec{r}\,'_8)\, \delta(s_8, s'_8)\, \delta(t_8, t'_8) \end{vmatrix}$$

$$\times\ d\tau\ \mathcal{O}\, G_{N\ell m}(\vec{r}_1 \ldots \vec{r}_8)\, X(S, T)\, d\tau \qquad \ldots(28)$$

and N^2 is equal to the right hand side of the above equation with $\mathcal{O} = 1$. Recalling the expression for the charge-spin function on page 22 it follows that after performing the summation over the spin coordinates equation (28) becomes

$$N^2 \langle \mathcal{O} \rangle = \iint G_{N\ell m}\,(\vec{r}\,'_1 \ldots . \vec{r}\,'_8)^*$$

$$\begin{vmatrix}
\delta(\vec{r}_1-\vec{r}\,'_1) & 0 & 0 & 0 & \delta(\vec{r}_1-\vec{r}\,'_5) & 0 & 0 & 0 \\
0 & \delta(\vec{r}_2-\vec{r}\,'_2) & 0 & 0 & 0 & \delta(\vec{r}_2-\vec{r}\,'_6) & 0 & 0 \\
0 & 0 & \delta(\vec{r}_3-\vec{r}\,'_3) & 0 & 0 & 0 & \delta(\vec{r}_3-\vec{r}\,'_7) & 0 \\
0 & 0 & & \delta(\vec{r}_4-\vec{r}\,'_4) & 0 & 0 & 0 & \delta(\vec{r}_4-\vec{r}\,'_8) \\
\delta(\vec{r}_5-\vec{r}\,'_1) & 0 & 0 & 0 & \delta(\vec{r}_5-\vec{r}\,'_5) & 0 & 0 & 0 \\
0 & \delta(\vec{r}_6-\vec{r}\,'_2) & 0 & 0 & 0 & \delta(\vec{r}_6-\vec{r}\,'_6) & 0 & 0 \\
0 & 0 & \delta(\vec{r}_7-\vec{r}\,'_3) & 0 & 0 & 0 & \delta(\vec{r}_7-\vec{r}\,'_7) & 0 \\
0 & 0 & 0 & \delta(\vec{r}_8-\vec{r}\,'_4) & 0 & 0 & 0 & \delta(\vec{r}_8-\vec{r}\,'_8)
\end{vmatrix}$$

$$\times\ d\tau'\, \mathcal{O}\, G_{N\ell m}(\vec{r}_1 \ldots \vec{r}_8)\ d\tau \qquad \ldots(29)$$

The integration sign no longer includes a summation over the spin coordinates. In Appendix 10 it is shown that, as far as expectation values are concerned

$$\begin{vmatrix}
\delta(\vec{r}_1-\vec{r}\,'_1) & 0 & 0 & 0 & \delta(\vec{r}_1-\vec{r}\,'_5) & 0 & 0 & 0 \\
0 & \delta(\vec{r}_2-\vec{r}\,'_2) & 0 & 0 & 0 & \delta(\vec{r}_2-\vec{r}\,'_6) & 0 & 0 \\
0 & 0 & \delta(\vec{r}_3-\vec{r}\,'_3) & 0 & 0 & 0 & \delta(\vec{r}_3-\vec{r}\,'_7) & 0 \\
0 & 0 & 0 & \delta(\vec{r}_4-\vec{r}\,'_4) & 0 & 0 & 0 & \delta(\vec{r}_4-\vec{r}\,'_8) \\
\delta(\vec{r}_5-\vec{r}\,'_1) & 0 & 0 & 0 & \delta(\vec{r}_5-\vec{r}\,'_5) & 0 & 0 & 0 \\
0 & \delta(\vec{r}_6-\vec{r}\,'_2) & 0 & 0 & 0 & \delta(\vec{r}_6-\vec{r}\,'_6) & 0 & 0 \\
0 & 0 & \delta(\vec{r}_7-\vec{r}\,'_3) & 0 & 0 & 0 & \delta(\vec{r}_7-\vec{r}\,'_7) & 0 \\
0 & 0 & 0 & \delta(\vec{r}_8-\vec{r}\,'_4) & 0 & 0 & 0 & \delta(\vec{r}_8-\vec{r}\,'_8)
\end{vmatrix}$$

$$= 2(1-4P_{48} + 3P_{37}P_{48}) \quad \delta(\vec{r}_1-\vec{r}\,'_1) \ldots \delta(\vec{r}_8-\vec{r}\,'_8)$$

Substituting this identity into equation 29 yields,

$$\langle\theta\rangle = \frac{\iint G_{N\ell m}(\vec{r}'_1\ldots\vec{r}'_8)^*\left[1-4P_{48}+3P_{37}P_{48}\right]\delta(\vec{r}_1-\vec{r}'_1)\ldots\;\ldots\delta(\vec{r}_8-\vec{r}'_8)\,d\tau'\,\theta\,G_{N\ell m}(\vec{r}_1\ldots\vec{r}_8)\,d\tau}{\iint G_{N\ell m}(\vec{r}'_1\ldots\vec{r}'_8)^*\left[1-4P_{48}+3P_{37}P_{48}\right]\delta(\vec{r}_1-\vec{r}'_1)\ldots\;\ldots\delta(\vec{r}_8-\vec{r}'_8)\,d\tau'\,G_{N\ell m}(\vec{r}_1\ldots\vec{r}_8)\,d\tau}$$

Integrating over the primed coordinates gives

$$\langle\theta\rangle = \frac{\int\left\{\left[1-4P_{48}+3P_{48}P_{37}\right]G_{N\ell m}(\vec{r}_1\ldots\vec{r}_8)^*\right\}\theta\,G_{N\ell m}(\vec{r}_1\ldots\vec{r}_8)\,d\tau}{\int\left\{\left[1-4P_{48}+3P_{48}P_{37}\right]G_{N\ell m}(\vec{r}_1\ldots\vec{r}_8)^*\right\}G_{N\ell m}(\vec{r}_1\ldots\vec{r}_8)\,d\tau} \qquad \ldots(30$$

and finally simplifying the notation this becomes

$$\langle\theta\rangle = \frac{I_1 - 4I_2 + 3I_3}{I_4 - 4I_5 + 3I_6} \qquad \ldots(31)$$

where

$$\begin{aligned} I_1 &= \int\psi(o)^*\,\theta\,\psi(o)\,d\tau \;:\quad & I_2 &= \int\psi(48)^*\,\theta\,\psi(o)\,d\tau \\ I_3 &= \int\psi(37,48)^*\theta\,\psi(o)\,d\tau \;:\quad & I_4 &= \int\psi(o)^*\,\psi(o)\,d\tau \\ I_5 &= \int\psi(48)^*\,\psi(o)\,d\tau \;:\quad & I_6 &= \int\psi(37,48)^*\,\psi(o)\,d\tau \end{aligned} \qquad \ldots(32$$

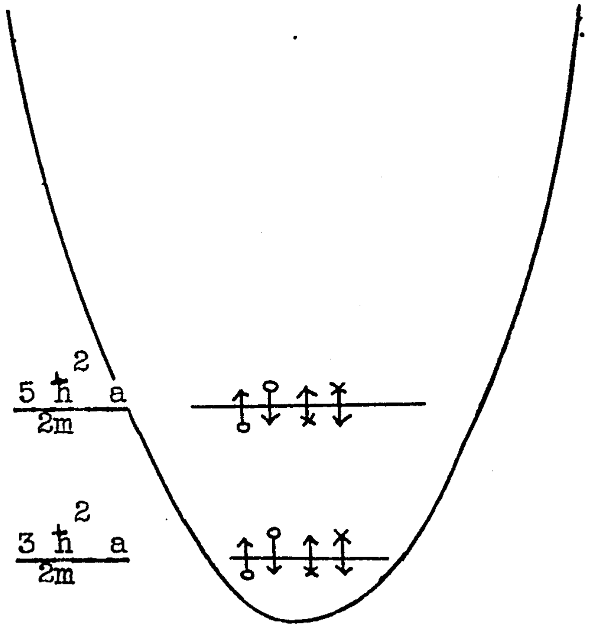
Each of these integrals involve an integration over 24 independent variables. In Appendix 12 they are reduced to a simple form.

Unfortunately the quantities of which the expectation value is being sought (ie. the r.m.s. cluster separation and cluster radius) are not invariant with respect to an interchange of any twonucleons. This leads one back to the basis of the cluster model to search for the terms most significant in the determination of the expectation value of these unsymmetrical dynamical operators.

It is clear that the requirement,of the cluster model wave function to be antisymmetric with respect to an interchange of any two nucleons, introduces the exchange integrals into the expectation values. That is, in order to insure no two nucleons will occupy the same quantum state and at the same time be indistinguishable, the exchange integrals are brought about. Hence, it is established that the problem is,"Which of the exchange integrals are the significant ones?".

Due to the close association of the cluster model with the independent particle model with an harmonic oscillator potential the incorporation of the exclusion principle and the indistinguishability requirement into the cluster model will be viewed in the light of this simple shell model. After all, the choice of the set of quantum numbers, (N,ℓ,m), describing the state of Be^8 was established by stabilizing the cluster model into the realm of the independent particle model through the incorporation of the exclusion principle. It is seen from figure 2 that in this simple

FIGURE 2



Simple shell model energy level picture of ^{8}Be in the ground state. The symbols, $\underset{\circ}{\uparrow}$, $\overset{\circ}{\downarrow}$, $\underset{\times}{\uparrow}$, $\overset{\times}{\downarrow}$, denote a proton with spin $\frac{1}{2}$, a proton with spin $-\frac{1}{2}$, a neutron with spin $\frac{1}{2}$, and a neutron with spin $-\frac{1}{2}$ respectively.

shell model the exclusion principle allows only four nucleons in the ground state.Furthermore it requires that two of the nucleons be protons with opposite intrinsic spin and two be neutrons with different intrinsic spin. Now consider the situation if it were required that the wave function be antisymmetric with respect to particles in the same charge spin state only. This would force nucleons with the same charge and spin into different energy levels and thus producing the same total energy of the system. Thus it is seen that the exclusion principle is completely satisfied. Hence it is seen by this example that requiring the wave function to be completely antisymmetric is a more strict requirement than the requirement that only the exclusion principle be obeyed.

In the above example the exclusion principle is obeyed but what what isn't obeyed and what makes this antisymmetrization approximation truly an approximation is that the wave function is neither completely symmetric nor completely antisymmetric. That is, with this approximation the wave function of the nucleus is of mixed symmetry. However, this is not possible for a proper formulation of a quantum mechanical description of indistinguishable particles. Thus, the above approximation satisfies the requirements of the exclusion principle but does not obey the more fundamental requirement of nature that the wave function of a system of fermions must be completely antisymmetric with respect to an interchange of any two of the particles.

Incidently this approximation of antisymmetrizing with respect to only particles in the same charge and spin state is not a new one in nuclear structure calculations. Perring and Skyrme (17) have made the following statement; "It seems to be true in general that it is only necessary to antisymmetrize with respect to particles with the same spin-charge function".

With the preceding discussion, it seems that it is appropiate to develop the analytical expression for the expected value of an operator subject to the foregoing approximation. With this approximation it follows from the original labeling of the particles that it is required that the wave function be antisymmetric with respect to an interchange of particles 1 and 5, 2 and 6, 3 and 7, and 4 and 8.

Before proceeding further it is instructive and later of use in the analyical work to introduce the following theorems and their corresponding proofs.

Theorem 1

If F is any function of the eight position vectors then

$$P_{15}(\mathcal{A}_{26}\mathcal{A}_{15}F) = -\mathcal{A}_{26}\mathcal{A}_{15}F \qquad --- (33)$$

for the cluster model of Be^8 given in this thesis. P_{15} denotes an operator that exchanges particles 1 and5, and $\mathcal{A}_{ij}$ denotes an operator that antisymmetrizes the operand with respect to particles "i" and "j".

Proof

$$\mathcal{A}_{26}\mathcal{A}_{15}\,F = \mathcal{A}_{26}\int F(\vec{r}\,'_1,\ldots\vec{r}\,'_8)\begin{vmatrix}\delta(\vec{r}_1-\vec{r}\,'_1) & \delta(\vec{r}_1-\vec{r}\,'_5)\\ \delta(\vec{r}_5-\vec{r}\,'_1) & \delta(\vec{r}_5-\vec{r}\,'_5)\end{vmatrix}\ \delta(\vec{r}_2-\vec{r}\,'_2)$$

$$\delta(\vec{r}_3-\vec{r}\,'_3)\,\delta(\vec{r}_4-\vec{r}\,'_4)\,\delta(\vec{r}_6-\vec{r}\,'_6)\,\delta(\vec{r}_7-\vec{r}\,'_7)\,\delta(\vec{r}_8-\vec{r}\,'_8)\quad d\tau'$$

$$= \mathcal{A}_{26}(F - P_{15}F) = \quad (1-P_{26})(1-P_{15})\,F$$

$$= F(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_6,\vec{r}_7,\vec{r}_8) - F(\vec{r}_5,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_1,\vec{r}_6,\vec{r}_7,\vec{r}_8)$$

$$- F(\vec{r}_1,\vec{r}_6,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_2,\vec{r}_7,\vec{r}_8) - F(\vec{r}_5,\vec{r}_6,\vec{r}_3,\vec{r}_4,\vec{r}_1,\vec{r}_2,\vec{r}_7,\vec{r}_8)$$

Then

$$P_{15}(\mathcal{A}_{26}\mathcal{A}_{15}\,F) = F(\vec{r}_5,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_1,\vec{r}_6,\vec{r}_7,\vec{r}_8) - F(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_6,$$

$$\vec{r}_7,\vec{r}_8) - F(\vec{r}_5,\vec{r}_6,\vec{r}_3,\vec{r}_4,\vec{r}_1,\vec{r}_2,\vec{r}_7,\vec{r}_8) + F(\vec{r}_1,\vec{r}_6,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_2,\vec{r}_7,\vec{r}_8)$$

$$= -\mathcal{A}_{26}\mathcal{A}_{15}F$$

Theorem 2

If F is any function of the eight position vectors then in general

$$P_{12}(\mathcal{A}_{16}\mathcal{A}_{12}F) \neq -\mathcal{A}_{16}\mathcal{A}_{12}F \qquad ----(34)$$

for the cluster model of Be^8.

Proof

It follows from the last theorem that

$$\mathcal{A}_{16}\mathcal{A}_{12}F = (1 - P_{16} - P_{12} + P_{16}P_{12})F$$

$$= F(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_6,\vec{r}_7,\vec{r}_8) - F(\vec{r}_6,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_1,\vec{r}_7,\vec{r}_8)$$

$$- F(\vec{r}_2,\vec{r}_1,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_6,\vec{r}_7,\vec{r}_8) + F(\vec{r}_2,\vec{r}_6,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_1,\vec{r}_7,\vec{r}_8)$$

Then

$$P_{12}(\mathcal{A}_{16}\mathcal{A}_{12}F) = F(\vec{r}_2,\vec{r}_1,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_6,\vec{r}_7,\vec{r}_8) - F(\vec{r}_6,\vec{r}_1,\vec{r}_3,\vec{r}_4,\vec{r}_5,$$

$$\vec{r}_2,\vec{r}_7,\vec{r}_8) - F(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_6,\vec{r}_7,\vec{r}_8) + F(\vec{r}_1,\vec{r}_6,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_2,\vec{r}_7,\vec{r}_8)$$

$$\neq -\mathcal{A}_{16}\mathcal{A}_{12}F$$

Returning to the development of the analytical expression for the expected value of an operator when the wave function is only antisymmetrized with respect to particles with the same charge-spin function it is seen almost immediately that after the summation over the charge-spin coordinates

$$N^2\langle \mathcal{O}\rangle = \frac{1}{2^4}\int (1-P_{15})(1-P_{26})(1-P_{37})(1-P_{48})\,G_{N\ell m}(\vec{r}_1..\vec{r}_8)^*$$

$$\mathcal{O}(1-P_{15})(1-P_{26})(1-P_{37})(1-P_{48})G_{N\ell m}(\vec{r}_1..\vec{r}_8)$$

But it is found in Appendix 10 that with respect to the cluster model wave function of Be^8 in the ground state (and also the first two excited states)

$$(1-P_{15})(1-P_{26})(1-P_{37})(1-P_{48}) = 2(1-P_{26}-P_{15}-P_{37}-P_{48}+P_{48}P_{37}+P_{37}P_{26}+P_{48}P_{26})$$

Therefore

$$N^2\langle\mathcal{O}\rangle = \frac{1}{4}\int d\tau\Big\{\Psi(o)^* - \Psi(15)^* - \Psi(26)^* - \Psi(37)^* - \Psi(48)^* + \Psi(48,37)^* + \Psi(37,26)^* + \Psi(48,26)^*\Big\}\mathcal{O}\Big\{\Psi(o) - \Psi(15) - \Psi(26) - \Psi(37) - \Psi(48) + \Psi(48,37) + \Psi(37,26) + \Psi(48,26)\Big\}$$

After utilizing certain symmetry properties it follows for a non-differential operator that in the ground state(and also for the excited states when m = 0) the preceding equation reduces to

$$\langle \mathcal{O} \rangle = \frac{1}{2}_{3} \; \frac{I_1 - 8I_2 + 6I_3 + 4I_{10} + 12I_{11} - 24I_{12} + 3I_{13} + 6I_{14}}{I_4 - 4I_5 + 3I_6} \quad \text{---(36)}$$

where

$I_1 = \int \psi(0)\mathcal{O}\psi(0)\,d\tau$ $\qquad$ $I_2 = \int \psi(0)\mathcal{O}\psi(48)\,d\tau$

$I_3 = \int \psi(0)\mathcal{O}\psi(48,37)\,d\tau$ $\qquad$ $I_4 = \int \psi(0)\mathcal{O}\psi(0)\,d\tau$

$I_5 = \int \psi(0)\mathcal{O}\psi(48)\,d\tau$ $\qquad$ $I_6 = \int \psi(0)\mathcal{O}\psi(48,37)\,d\tau$

$I_{10} = \int \psi(48)\mathcal{O}\psi(48)\,d\tau$ $\qquad$ $I_{11} = \int \psi(48)\mathcal{O}\psi(37)\,d\tau$

$I_{12} = \int \psi(26)\mathcal{O}\psi(48,37)\,d\tau$ $\qquad$ $I_{13} = \int \psi(48,37)\mathcal{O}\psi(48,37)\,d\tau$

$I_{14} = \int \psi(48,37)\mathcal{O}\psi(48,26)\,d\tau$

Before considering the effects of this approximation it is again instructive and later useful to introduce theorems 3 and 4 and their proofs.

Theorem 3

The expectation value of an operator that is antisymmetric with respect to an interchange of particles is zero.

Proof

Suppose operator, $\mathcal{O}$, is antisymmetric in all particles.

Then $\mathcal{O}\psi_{N\ell m} = \mathcal{O}\mathcal{A}G_{N\ell m}X = S(\mathcal{O}G_{N\ell m}X)$

Furthermore if u and v are any functions of the eight position vectors that are ,in general, neither symmetric nor antisymmetric

$$(\mathcal{A}u)(\mathcal{S}v) = \mathcal{A}(u(\mathcal{S}v))$$

for if $fn = (\mathcal{S}v)u$ then it is clear that

$$\mathcal{A}\,fn = \mathcal{A}(u(\mathcal{S}v)) = (\mathcal{S}v)(\mathcal{A}u)$$

Hence

$$\langle\mathcal{O}\rangle = \int\psi^{*}_{N\ell m}\mathcal{O}\psi_{N\ell m}\,d\tau = \int\mathcal{A}(G_{N\ell m}X)^{*}\,\mathcal{S}(\mathcal{O}G_{N\ell m}X)\,d\tau$$

$$= \int\mathcal{A}(G^{*}_{N\ell m}X\,(\mathcal{S}\mathcal{O}G_{N\ell m}X))\,d\tau = \int\mathcal{A}(G^{*}_{N\ell m}X\mathcal{O}\mathcal{S}G_{N\ell m}X)\,d\tau$$

But the integral of an antisymmetric function over all space is zero.This can be seen by considering any antisymmetric function fn, for

$$\int\mathcal{A}\,fn(\vec{r}_1\ldots\vec{r}_N)\,d\vec{r}_1\ldots d\vec{r}_N = \frac{1}{\sqrt{N!}}\int fn(\vec{r}\,'_1\ldots\vec{r}\,'_N)\begin{vmatrix}\delta(\vec{r}_1-\vec{r}\,'_1)\ldots\delta(\vec{r}_1-\vec{r}\,'_N)\\ \delta(\vec{r}_N-\vec{r}\,'_1)\ldots\delta(\vec{r}_N-\vec{r}\,'_N)\end{vmatrix}$$

$$d\vec{r}_1\ldots d\vec{r}_N\,d\vec{r}\,'_1\ldots d\vec{r}\,'_N$$

Integrating over the unprimed clearly yields a zero value. Hence the expectation value of an antisymmetric operator is zero.

Theorem 4

Suppose $\mathcal{O}$ is a symmetric operator with respect to an interchange of any two particles and the wave functions ψ_1 and ψ_2 can assume any one of the three possible forms $\psi(o)$, $\psi(ij)$, and $\psi(ij,lm)$ and i,j,ℓ, and m can assume any integer of the set from 1 to 8. Then all integrals of the form

$$\int \psi_1^* \mathcal{O} \psi_2 \, d\tau$$

are invariant under any exchange operation, P_{ij}, on the complete integrand for all nine possible combinations of ψ_1 and ψ_2.

Proof

Consider the integral

$$I = \int \psi(ij)^* \mathcal{O} \psi(nm,k\ell) d\tau$$

Since operator $\mathcal{O}$ is symmetrical under interchange of any two particles then

$$I = \int P_{k\ell} \left\{ \psi(ij,k\ell)^* \mathcal{O} \psi(nm) \right\} d\tau$$

where $P_{k\ell}$ is the exchange operator which interchanges particles k and ℓ. But it is easily seen that

$$P_{k\ell} = 1 - \mathcal{A}_{k\ell}$$

where $\mathcal{A}_{k\ell}$ is an operator which antisymmetrizes it's operand with respect to particles k and ℓ. Therefore

$$I=\int \psi(ij,k\ell)^{*}\,\mathcal{O}\,\psi(nm)\,d\tau \;-\; \int A_{k\ell}\left\{\psi(ij,k\ell)^{*}\,\mathcal{O}\,\psi(nm)\right\} d\tau$$

However by theorem 3 the second integral in the above expression is zero. Hence

$$\int \psi(ij)^{*}\,\mathcal{O}\,\psi(nm,k\ell)\,d\tau=\int \psi(ij,k\ell)^{*}\,\mathcal{O}\,\psi(nm)\,d\tau$$

Similarly for all other combinations.

A further insight into the approximation involved when the wave function is antisymmetrized only with respect to particles with the same charge-spin function will now be obtained by the following theorem. This is an important theorem, for the Hamiltonian of a system of nucleons is, in general, symmetrical.

Theorem 5

In the cluster model of Be^{8} the approximation involved by assuming it necessary to antisymmetrize only with respect to nucleons in the same charge spin state is strictly valid, in the ground state, in the determination of the expected value of a symmetrical dynamical operator with the magnitude of discrepancy being zero.

Proof

It follows from equation 35 for the expectation value of an operator in the ground state of the cluster model of Be^{8} that for the more general case of possible differential operators

$$N^{2}\langle\mathcal{O}\rangle = \frac{1}{2^{2}}\Big\{ I_{1} - 4I_{2} + 3I_{3} - 4I_{15} + 4I_{10} + 3I_{17} - 6I_{12} + 12I_{11} - 6I_{16} - 6I_{18} - 6I_{19} + 3I_{13} + 6I_{14} \Big\} \quad ---- (37)$$

where

$$I_{15} = \int \psi(26)^{*}\mathcal{O}\psi(o)\,d\tau \qquad I_{16} = \int \psi(26)^{*}\mathcal{O}\psi(37,26)\,d\tau$$

$$I_{17} = \int \psi(48,37)^{*}\mathcal{O}\psi(o)\,d\tau \qquad I_{18} = \int \psi(48,37)^{*}\mathcal{O}\psi(26)\,d\tau$$

$$I_{19} = \int \psi(48,37)^{*}\mathcal{O}\psi(37)\,d\tau$$

It is shown on page 38 that if operator, $\mathcal{O}$, is symmetrical (ie.invariant with respect to an interchange of any two nucleons) then,

$$N^{2}\langle\mathcal{O}\rangle = I_{1} - 4I_{2} + 3I_{3}$$

Hence to show that the discrepancy introduced by the approximation in the wave function antisymmetrization is of zero magnitude for symmetrical operators it is required to show that

$$7I_{1} - 28I_{15} + 21I_{17} - 3I_{3} + 4I_{2} - 4I_{10} - 12I_{11} + 6I_{12} + 6I_{16} + 6I_{18} + 6I_{19} - 3I_{13} - 6I_{14} = 0$$

However it follows from theorem 4 that

$$I_{17} = I_3 , I_{15} = I_2 , I_{10} = I_1 , I_{12} = I_2$$

$$I_{13} = I_1 , I_{16} = I_2 , I_{18} = I_2 , I_{19} = I_2$$

$$I_{11} = I_3 , I_{14} = I_3$$

for symmetrical operators. Hence the theorem is proved.

It follows from theorem 5 that this approximation in the wave function antisymmetrization is strictly correct for ground state energy level calculations. It can be noted however, that the approximation adds nothing to the simplication of these calculations.

Corollary

For the determination of the expected value of quantum mechanical operators, symmetrical under the interchange of any two nucleons(such as the determination of energy levels), in the cluster model of the Be^8 nucleus it is sufficient to satisfy Pauli's exclusion principle in the frame of the simple shell model and not necessary to satisfy the more fundamental requirement of nature that the wave function be antisymmetric.

Theorem 6

In the excited states of the cluster model the expectation value of a symmetrical operator(such as a hamiltonian operator) void of exchange effects can be determined from the unantisymmetrized wave function.

Proof

The proof is seen from theorem 5 and from the fact that spherical harmonic functions are orthogonal.

It follows from theorem 6 that,in the excited states, the energy levels corresponding to a hamiltonian operator free from exchange effects can be described by an unantisymmetrized cluster model wave function. That is, the exchange integrals arising in the expression for this type of operator vanish in the excited states. Thus, as far as the energy levels corresponding to a hamiltonian free of exchange effects is concerned, in it's excited states the nucleus is behaving as though it consisted of two distinct alpha particles with no exchange of nucleons between the clusters. This raises the question,"Does this mean that,under these conditions, there exists no real exchange of nucleons between the clusters"?Just because one finds that there is no exchange effects in the expectation values of the energy in the excited states it wouldn't be possible to conclude that this means that there is no exchange of nucleons taking place. This is seen from the non-zero values of the exchange integrals for unsymmetrical operators.

The advantage of considering this unrealistic hamiltonian is that some insight may be gained about the effect of the exchange terms that do arise in a real hamiltonian.

2. Cluster Radius and Separation

It is shown in Appendix 4 that the following quantity

$$\sum_{i=1}^{8} \gamma_i^2 + 2R^2$$

is invariant with respect to an interchange of any two nucleons. Hence it is possible to find the expected value of the above quantity through the simple formalism for symmetrical operators given on page 38.This suggests the following algorithm for the determination of the shape of Be^8.

Step 1

Determine exactly

$$4\langle \gamma^2 \rangle + \langle R^2 \rangle$$

through the application of the symmetrical operator formalism.

Step 2

Determine the approximate expected value of the square of the relative alpha cluster separation with the wave function which is only antisymmetric with respect to particles in the same charge spin state

Step 3

The expectation of the square of the cluster separtion is found from the results of steps 1 and 2.

Before proceding it will be recalled that the energy of the nuclear system subject to the approximation in step 2 is the same as the correct value and furthermore,although the wave function is not completely antisymmetric the exclusion principle is satisfied.

Denoting the expected value of the square of the relative separation when calculated in the framework for symmetrical operators by $\left\langle R^2_{sf} \right\rangle$, it follows

$$\left\langle R^2_{sf} \right\rangle_{N\ell m} = \frac{\int \psi^*_{N\ell m} R^2 \psi_{N\ell m} \, d\tau}{\int \psi^*_{N\ell m} \psi_{N\ell m} \, d\tau}$$

It is seen from Appendix 12 that

$$\left\langle R^2_{sf} \right\rangle_{N\ell m} = \frac{I(R^2)_1 - 4I(R^2)_2 + 3I(R^2)_3}{I_4 - 4I_5 + 3I_6}$$

and this reduces to

$$\left\langle R^2_{sf} \right\rangle = \frac{\mathcal{F}(2\beta) - 2^8\left[\frac{a}{6\pi}\right]^{\frac{3}{2}} \mathcal{J}\left(\frac{5a}{3}+\beta, \frac{8a}{3}, \frac{5a}{3}+\beta\right) + 3\cdot 2^3\left[\frac{a}{2\pi}\right]^{\frac{3}{2}} \mathcal{J}(a+\beta, 0, a+\beta)}{I(2\beta) - 2^8\left[\frac{a}{6\pi}\right]^{\frac{3}{2}} J\left(\frac{5a}{3}+\beta, \frac{8a}{3}, \frac{5a}{3}+\beta\right) + 3\cdot 2^3\left[\frac{a}{2\pi}\right]^{\frac{3}{2}} J(a+\beta, 0, a+\beta)}$$

where

$$I(p) = \int_0^\infty R^{2N+2} \exp\left[-pR^2\right] dR$$

$$J(p,q,s) = \int R'^{N+2} R^{N+2} \exp\left[-pR'^2 + qR'\cdot R - sR^2\right] Y_\ell^m(\Omega) Y_\ell^m(\Omega') \, dR \, dR' \, d\Omega' \, d$$

$$\mathcal{F}(p) = \int_0^\infty R^{2N+4} \exp\left[-pR^2\right] dR$$

$$\mathcal{Q}(p,q,s) = \int R'^{N+2} R^{N+4} \exp\left[-pR'^2 + qR'\cdot R - sR^2\right] Y_\ell^m(\Omega) Y_\ell^m(\Omega')\, dR\, dR'\, d\Omega\, d\Omega'$$

These integrals have been evaluated analyically in Appendix 17 and 18. The expectation value can now be written

$$a\left\langle R^2_{sf}\right\rangle_{N\ell m} = \frac{\mathcal{F}(2\varepsilon) - 2^8\left[\frac{1}{6\pi}\right]^{\frac{3}{2}} \mathcal{Q}\left(\frac{5}{3}+\varepsilon, \frac{8}{3}, \frac{5}{3}+\varepsilon\right) + 3\cdot 2^3 \left[\frac{1}{2\pi}\right]^{\frac{3}{2}} \mathcal{Q}(1+\varepsilon, 0, 1+\varepsilon)}{I(2\varepsilon) - 2^8\left[\frac{1}{6\pi}\right]^{\frac{3}{2}} J\left(\frac{5}{3}+\varepsilon, \frac{8}{3}, \frac{5}{3}+\varepsilon\right) + 3\cdot 2^3 \left[\frac{1}{2\pi}\right]^{\frac{3}{2}} J(1+\varepsilon, 0, 1+\varepsilon)}$$

where in the ground state

$$\mathcal{F}(2\varepsilon) \quad \frac{11\cdot 9\cdot 7\cdot 5\cdot 3\sqrt{\pi}}{2^{13+\frac{1}{2}}\,\varepsilon^{6+\frac{1}{2}}}$$

$$\mathcal{Q}\left(\frac{5}{3}+\varepsilon, \frac{8}{3}, \frac{5}{3}+\varepsilon\right) = \frac{7\cdot 5\cdot 3^{5+\frac{1}{2}}\,\pi^2\,(5+3\varepsilon)}{2^7\,(3+10\varepsilon+3\varepsilon^2)^{4+\frac{1}{2}}}\left[5 + \frac{5\cdot 2^5}{(3+10\varepsilon+3\varepsilon^2)} + \frac{11\cdot 2^8}{3(3+10\varepsilon+3\varepsilon^2)^2}\right]$$

$$\mathcal{Q}(1+\varepsilon, 0, 1+\varepsilon) = \frac{5^2\cdot 3^2\cdot 7\cdot\pi^2}{2^7\,(1+\varepsilon)^8}$$

$$I(2\varepsilon) = \frac{9\cdot7\cdot5\cdot3\sqrt{\pi}}{2^{11+\frac{1}{2}}\,\varepsilon^{5+\frac{1}{2}}}$$

$$J\left(\frac{5}{3}+\varepsilon,\frac{8}{3},\frac{5}{3}+\varepsilon\right) = \frac{5\cdot3^{4+\frac{1}{2}}\,\pi^{2}}{2^{6}\,(3+10\varepsilon+3\varepsilon^{2})^{3+\frac{1}{2}}}\left[\,5\cdot3 + \frac{7\cdot5\cdot2^{5}}{3(3+10\varepsilon+3\varepsilon^{2})} + \frac{7\cdot2^{8}}{(3+10\varepsilon+3\varepsilon^{2})^{2}}\right]$$

$$J(1+\varepsilon,0,1+\varepsilon) = \frac{15^{2}\,\pi^{2}}{2^{6}\,(1+\varepsilon)^{7}}$$

The expectation values have been evaluated for various values of ε and the results are tabulated in table 1 and plotted as a function of ε in figure 2.

The next problem which is considered is the calculation of the expected square of the alpha cluster radius within the symmetrical operator framework. Without loss of generality the expectation of γ_8^2 will be evaluated in this framework. The $\langle\gamma_{sf}^2\rangle$ will denote the expected square of the alpha cluster radius calculated in the symmetrical operator framework. This expected value will be determined as a function of the variational parameters that appear in the generalized cluster model wave functions for Be^8. For the definition of $\vec{\gamma}_i$ see equation 8 page 11. We have that

$$\left\langle \gamma^{2}_{sf} \right\rangle_{N\ell m} = \frac{\int \psi^{*}_{N\ell m}\, \gamma^{2}_{8}\, \psi_{N\ell m}\, d\tau}{\int \psi^{*}_{N\ell m}\, \psi_{N\ell m}\, d\tau}$$

where the wave functions are antisymmetrized only with respect to nucleons in the same charge-spin state. Employing the results of the preceding work in this chapter we have that

$$\left\langle \gamma^{2}_{sf} \right\rangle = \frac{I(\gamma^{2}_{8})_{7} - 4I(\gamma^{2}_{8})_{8} + 3I(\gamma^{2}_{8})_{9}}{I_{4} - 4I_{5} + 3I_{6}}$$

where

$$I_{7} = \int \psi(0)\, \gamma^{2}_{8}\, \psi(0)\, d\tau \qquad I_{8} = \int \psi(48)\, \gamma^{2}_{8}\, \psi(0)\, d\tau$$

$$I_{9} = \int \psi(37,48)\, \gamma^{2}_{8}\, \psi(0)\, d\tau$$

It now follows from Appendices 19,22,and 24 that

$$a \left\langle \gamma^{2}_{sf} \right\rangle = \frac{1}{\pi^{9}\, 2^{6}} \left[\frac{I'_{7} - 4I'_{8} + 3I'_{9}}{I(2) - 2^{8}\left[\frac{a}{6\pi}\right]^{1+\frac{1}{2}} J\left(\frac{5}{3}+\varepsilon, \frac{8}{3}, \frac{5}{3}+\varepsilon\right) + 3\cdot 2^{3}\left[\frac{a}{2\pi}\right]^{1+\frac{1}{2}} J(1+\varepsilon, 0, 1+\varepsilon)} \right]$$

where

$$I'_{7} = \frac{3^{5}\cdot 7\cdot 5\, \pi^{9+\frac{1}{2}}}{2^{5+\frac{1}{2}}\, \varepsilon^{5+\frac{1}{2}}}$$

$$I'_8 = 2^{6+\frac{1}{2}} \cdot \pi^{7+\frac{1}{2}} \cdot 3^{\frac{1}{2}} \left[J\left(\frac{5}{3}+\varepsilon, \frac{8}{3}, \frac{5}{3}+\varepsilon\right) + \frac{2^5}{3^2} \mathcal{L}\left(\frac{5}{3}+\varepsilon, \frac{8}{3}, \frac{5}{3}+\varepsilon\right) - \frac{2^5}{3^2} T\left(\frac{5}{3}+\varepsilon, \frac{8}{3}, \frac{5}{3}+\varepsilon\right) \right]$$

$$I'_9 = 2^{5+\frac{1}{2}} \pi^{7+\frac{1}{2}} \left[\frac{5 \cdot 3}{2^2} J(1+\varepsilon, 0, 1+\varepsilon) + \mathcal{L}(1+\varepsilon, 0, 1+\varepsilon) \right]$$

In Appendix 21 it is shown that

$$T\left(\frac{5}{3}+\varepsilon, \frac{8}{3}, \frac{5}{3}+\varepsilon\right) = \frac{7^2 \cdot 5^2 \cdot 3^{4+\frac{1}{2}} \pi^2}{2^5 (3+10\varepsilon+3\varepsilon^2)^{4+\frac{1}{2}}} \left[1 + \frac{3 \cdot 2^5}{5(3+10\varepsilon+3\varepsilon^2)} + \frac{11 \cdot 2^8}{5 \cdot 7 (3+10\varepsilon+3\varepsilon^2)^2} \right]$$

With this expression the value of the product of the r.m.s. radius, determined within the framework of symmetrical operators, and $\sqrt{a}$ has been calculated and plotted as a function of ε for the ground state. The quantity $4\langle \gamma^2 \rangle + \langle R^2 \rangle$ is tabulated in table 3 and plotted in figure 5.

Now the value of the expectation of the square of the relative alpha cluster separation is determined with a wave function which isantisymmetric with respect to particles in the same charge-spin state. It follows from page48 and the results of Appendix 12 that

$$a\left\langle R^{2}\right\rangle \quad \frac{1}{\pi^{9}\,2^{9}}\left[\frac{I'_{1}-8I'_{2}+6I'_{3}+4I'_{10}+12I'_{11}-24I'_{12}+3I'_{13}+6I'_{14}}{I(2\varepsilon)-2^{8}\left[\frac{a}{6\pi}\right]^{1+\frac{1}{2}}J\left(\frac{5}{3}+\varepsilon,\frac{8}{3},\frac{5}{3}+\varepsilon\right)+3\cdot 2^{3}\left[\frac{1}{2\pi}\right]^{1+\frac{1}{2}}J(1+\varepsilon,0,1+\varepsilon}\right.$$

where now

$$I'_{1}=\pi^{9}\,2^{6}\,\mathcal{J}(2\varepsilon)$$

$$I'_{2}=2^{12}\left[\frac{\pi^{5}}{6}\right]^{1+\frac{1}{2}}\mathcal{L}\left(\frac{5}{3}+\varepsilon,\frac{8}{3},\frac{5}{3}+\varepsilon\right)$$

$$I'_{3}=2^{7+\frac{1}{2}}\,\pi^{7+\frac{1}{2}}\,\mathcal{L}(1+\varepsilon,0,1+\varepsilon)$$

$$I'_{10}=\frac{2^{10+\frac{1}{2}}\,\pi^{7+\frac{1}{2}}}{3}\quad A\left(\frac{2}{3}+2\varepsilon,\frac{8}{3},\frac{8}{3}\right)$$

$$I'_{11}=3\cdot 2^{\substack{3\\1+\frac{1}{2}}}\,\pi^{7+\frac{1}{2}}\left[J(1+\varepsilon,0,1+\varepsilon)+\frac{4}{3}\mathcal{L}(1+\varepsilon,0,1+\varepsilon)\right]$$

$$I'_{12}=\frac{2^{6+\frac{1}{2}}\,\pi^{7+\frac{1}{2}}}{3^{3+\frac{1}{2}}}\left[3^{2}J\left(\frac{5}{3}+\varepsilon,\frac{8}{3},\frac{5}{3}+\varepsilon\right)+10\mathcal{L}\left(\frac{5}{3}+\varepsilon,\frac{8}{3},\frac{5}{3}+\varepsilon\right)\right.$$

$$\left.-2^{3}\,T\left(\frac{5}{3}+\varepsilon,\frac{8}{3},\frac{5}{3}+\varepsilon\right)\right]$$

$$I'_{13} = \frac{3^4 \cdot 7 \cdot 5\, \pi^{9+\frac{1}{2}}}{2^{7+\frac{1}{2}}\, \varepsilon^{5+\frac{1}{2}}}$$

$$I'_{14} = \frac{3^3 \cdot 5^2\, \pi^{9+\frac{1}{2}}}{2^{3+\frac{1}{2}}\, (1+\varepsilon)^7}$$

and

$$A\left(\frac{2}{3} + 2\varepsilon, \frac{8}{3}, \frac{8}{3}\right) = \frac{7 \cdot 5 \cdot 3^{8+\frac{1}{2}}\, \pi^2}{2^{25}\, \varepsilon^{2+\frac{1}{2}}\, (1+3\varepsilon)^3} \left[3 + \frac{5}{3\varepsilon} + \frac{7}{3 \cdot 2^3\, \varepsilon^2} + \frac{1}{2^4 \cdot 3\, \varepsilon^3} + \frac{11}{3^4 \cdot 2^8\, \varepsilon^4} \right]$$

From this result the value of the product of the r.m.s. radius, determined with a wave function that is antisymmetric with respect to an interchange of nucleons in the same charge-spin state, and the square root of the width parameter "a" is computed and is plotted as a function of the ratio of the two width parameters, ε. Then from the values of $4\langle \gamma^2 \rangle + \langle R^2 \rangle$ the root mean square cluster radius is calculated as a function of a and ε. Next the degree of dumbbelledness of the Be^8 nucleus for the ground state according to the cluster model is calculated and plotted as a function of ε. The degree of dumbbelledness D_{400} is defined as the ratio of the r.m.s. expected cluster separation to the expected root mean square radius of the alpha clusters.

TABLE 1

R.M.S. CLUSTER SEPARATION DATA DETERMINED FROM SYMMETRICAL OPERATOR FRAMEWORK

ε	$\sqrt{\alpha}\sqrt{\langle R^2\rangle}$	ε	$\sqrt{\alpha}\sqrt{\langle R^2\rangle}$	ε	$\sqrt{\alpha}\sqrt{\langle R^2\rangle}$
.01	16.583	.41	2.777	.81	2.311
.02	11.726	.42	2.753	.82	2.307
.03	9.574	.43	2.730	.83	2.304
.04	8.292	.44	2.708	.84	2.301
.05	7.417	.45	2.687	.85	2.299
.06	6.771	.46	2.667	.86	2.296
.07	6.270	.47	2.648	.87	2.294
.08	5.866	.48	2.629	.88	2.292
.09	5.532	.49	2.612	.89	2.291
.10	5.250	.50	2.595	.90	2.290
.11	5.008	.51	2.578	.91	2.289
.12	4.800	.52	2.563	.92	2.288
.13	4.613	.53	2.548	.93	2.287
.14	4.450	.54	2.534	.94	2.287
.15	4.303	.55	2.520	.95	2.287
.16	4.171	.56	2.507	.96	2.288
.17	4.052	.57	2.494	.97	2.288
.18	3.943	.58	2.482	.98	2.289
.19	3.844	.59	2.470	.99	2.290
.20	3.753	.60	2.459	1.00	
.21	3.670	.61	2.448		
.22	3.592	.62	2.438		
.23	3.521	.63	2.428		
.24	3.454	.64	2.418		
.25	3.392	.65	2.409		
.26	3.335	.66	2.401		
.27	3.280	.67	2.392		
.28	3.230	.68	2.384		
.29	3.182	.69	2.377		
.30	3.137	.70	2.369		
.31	3.095	.71	2.362		
.32	3.055	.72	2.356		
.33	3.017	.73	2.350		
.34	2.981	.74	2.344		
.35	2.948	.75	2.338		
.36	2.915	.76	2.331		
.37	2.885	.77	2.328		
.38	2.856	.78	2.323		
.39	2.828	.79	2.319		
.40	2.802	.80	2.315		

FIGURE 3

The ground state, expected root mean square, separation of the alpha clusters in the Be^8 cluster model as determined from the symmetrical operator framework. The separation is given as a function of the variational parameters. $\sqrt{\langle R^2 \rangle_{N\ell m}}$ denotes the expected root mean square cluster separation in the nuclear state corresponding to the quantum numbers, $N\ell m$.

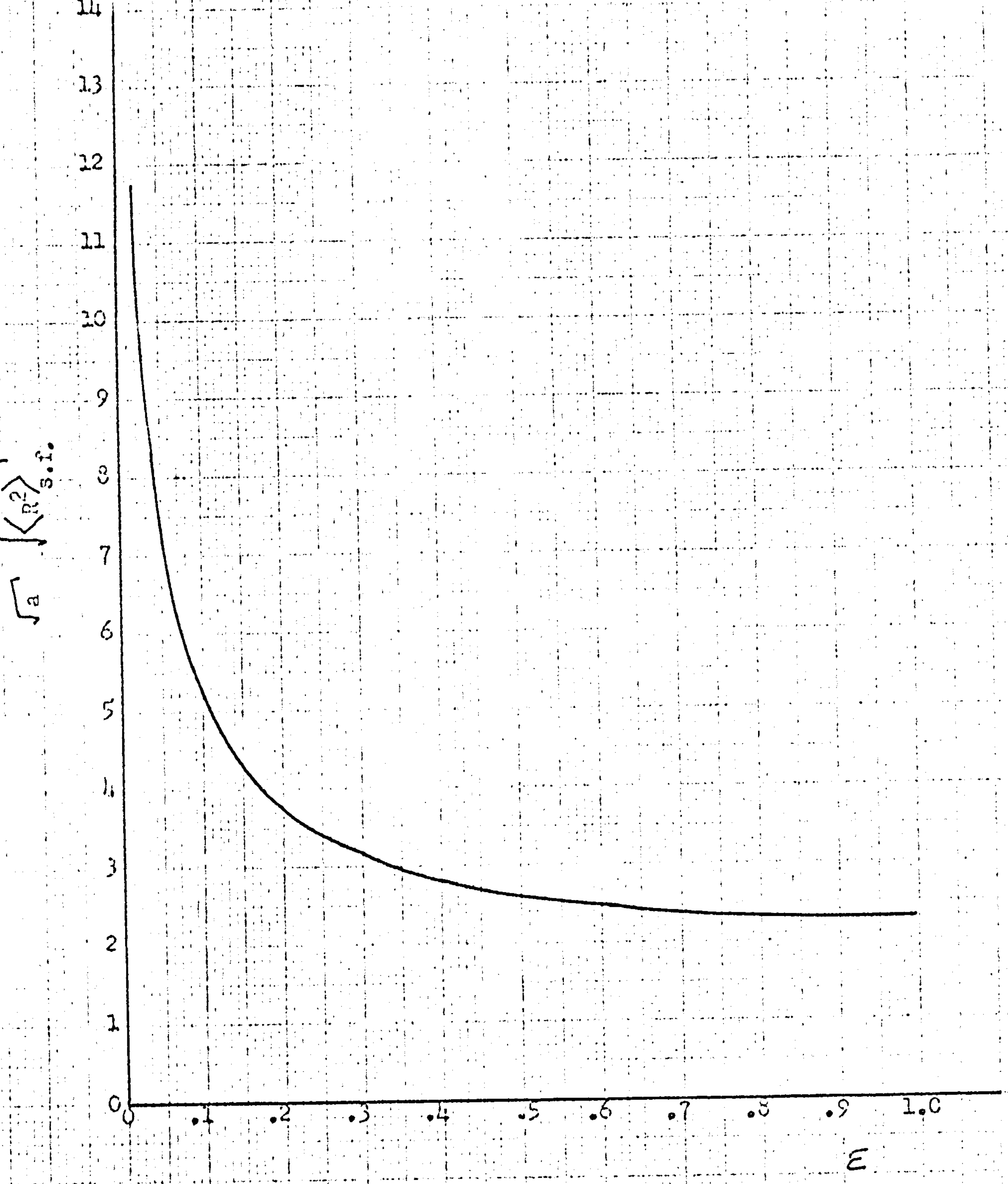

$\sqrt{a}\ \sqrt{\langle R^2\rangle_{s.f.}}$
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.0
ε

TABLE 2

R.M.S. CLUSTER RADIUS DATA DETERMINED FROM SYMMETRICAL OPERATOR FRAMEWORK

ε	$\sqrt{\alpha}\sqrt{\langle r^2\rangle}$
.01	3.000
.02	3.000
.03	3.000
.04	3.000
.05	3.000
.06	3.000
.07	3.001
.08	3.002
.09	3.003
.10	3.005
.11	3.007
.12	3.010
.13	3.013
.14	3.018
.15	3.023
.16	3.029
.17	3.036
.18	3.045
.19	3.054
.20	3.064
.21	3.076
.22	3.088
.23	3.102
.24	3.117
.25	3.133
.26	3.151
.27	3.169
.28	3.189
.29	3.210
.30	3.233
.31	3.256
.32	3.281
.33	3.308
.34	3.335
.35	3.364
.36	3.394
.37	3.426
.38	3.459
.39	3.493
.40	3.528
.41	3.565
.42	3.604
.43	3.644
.44	3.685
.45	3.728
.46	3.772
.47	3.818
.48	3.865
.49	3.914
.50	3.965
.51	4.017
.52	4.071
.53	4.127
.54	4.184
.55	4.243
.56	4.304
.57	4.367
.58	4.432
.59	4.499
.60	4.568
.61	4.639
.62	4.712
.63	4.788
.64	4.866
.65	4.946
.66	5.028
.67	5.114
.68	5.201
.69	5.292
.70	5.385
.71	5.481
.72	5.580
.73	5.682
.74	5.788
.75	5.896
.76	6.009
.77	6.124
.78	6.244
.79	6.367
.80	6.494
.81	6.626
.82	6.762
.83	6.902
.84	7.047
.85	7.197
.86	7.352
.87	7.512
.88	7.678
.89	7.850
.90	8.028
.91	8.212
.92	8.403
.93	8.601
.94	8.806
.95	9.019
.96	9.240
.97	9.469
.98	9.707
.99	9.954
1.00	

FIGURE 4

The ground state, expected root mean square, radius of the alpha clusters in the Be^8 cluster model as determined from the symmetrical operator framework. The separation is given as a function of the variational parameters. $\sqrt{\langle r^2\rangle_{N\ell m}}$ denotes the expected root mean square cluster radius in the nuclear state corresponding to the quantum numbers, $N\ell m$.

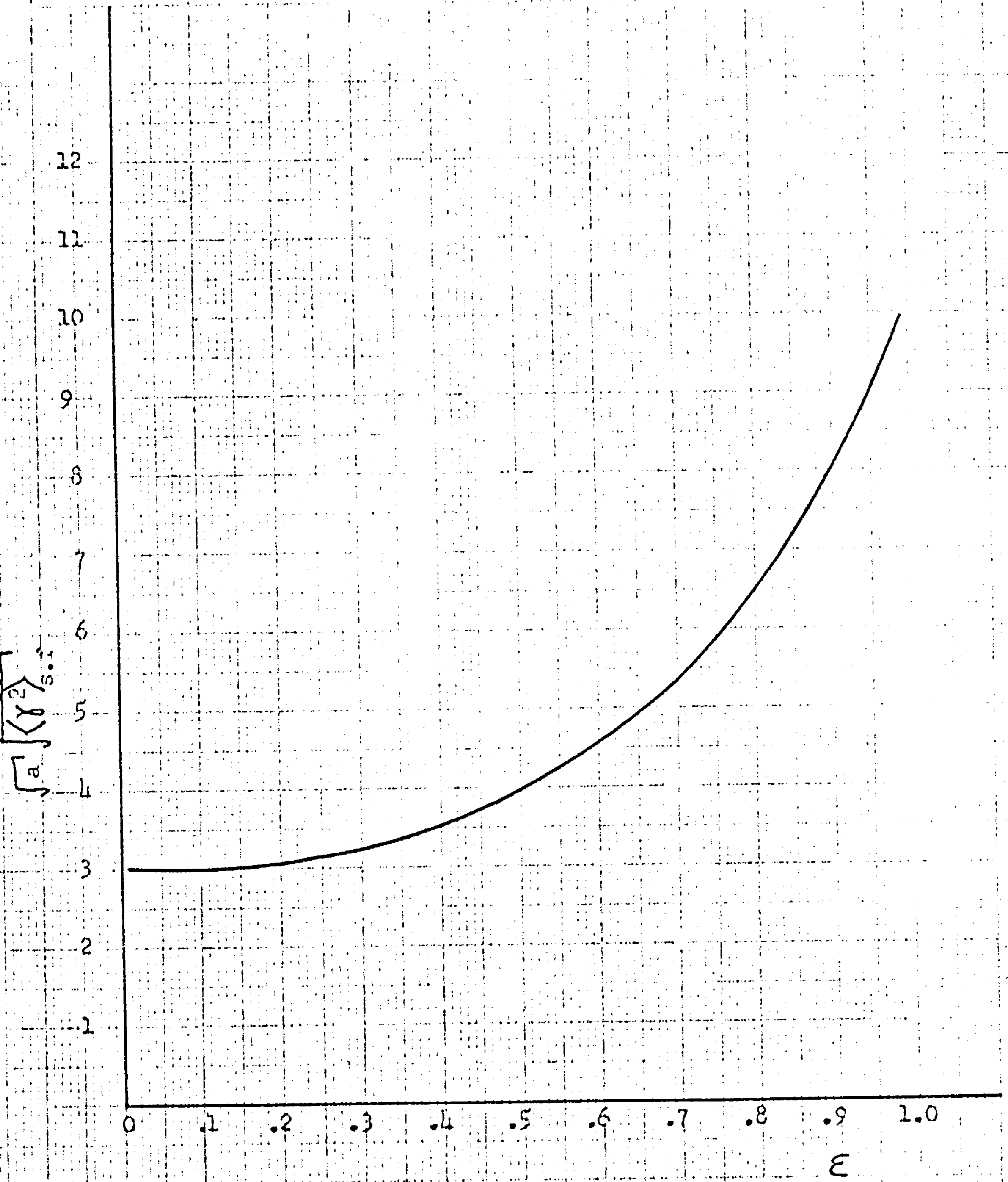

12
11
10
9
8
7
6
5
4
3
2
1
$\sqrt{a}\sqrt{\langle \gamma^2 \rangle_{s.i.}}$
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.0
ε

TABLE 3

DATA OF WEIGHTED SUM OF THE EXPECTED SQUARE OF ALPHA CLUSTER RADIUS AND SEPARATION

ε	$a[4\langle\gamma^2\rangle+\langle R^2\rangle]$
.01	311.0
.02	173.5
.03	127.7
.04	104.8
.05	91.0
.06	81.9
.07	75.3
.08	70.4
.09	66.7
.10	63.7
.11	61.2
.12	59.3
.13	57.6
.14	56.2
.15	55.1
.16	54.1
.17	53.3
.18	52.6
.19	52.1
.20	51.6
.21	51.3
.22	51.1
.23	50.9
.24	50.8
.25	50.8
.26	50.8
.27	50.9
.28	51.1
.29	51.4
.30	51.6
.31	52.0
.32	52.4
.33	52.9
.34	53.4
.35	54.0
.36	54.6
.37	55.3
.38	56.0
.39	56.8
.40	57.7
.41	58.6
.42	59.5
.43	60.6
.44	61.7
.45	62.8
.46	64.0
.47	65.3
.48	66.7
.49	68.1
.50	69.6
.51	71.2
.52	72.9
.53	74.6
.54	76.4
.55	78.4
.56	80.4
.57	82.5
.58	84.7
.59	87.1
.60	89.5
.61	92.1
.62	94.8
.63	97.6
.64	100.5
.65	103.6
.66	106.9
.67	110.3
.68	113.9
.69	117.7
.70	121.6
.71	125.8
.72	130.1
.73	134.7
.74	139.5
.75	144.5
.76	149.9
.77	155.4
.78	161.3
.79	167.5
.80	174.1
.81	180.9
.82	188.2
.83	195.9
.84	203.9
.85	212.5
.86	221.5
.87	231.0
.88	241.1
.89	251.8
.90	263.0
.91	275.0
.92	287.7
.93	301.2
.94	315.4
.95	330.6
.96	346.7
.97	363.9
.98	382.1
.99	401.6
1.00	

FIGURE 5

The weighted sum of the expected square of the alpha cluster radius and separation.

$$\text{Weighted Sum} = \alpha\left[4\langle \gamma^2 \rangle + \langle R^2 \rangle\right]$$

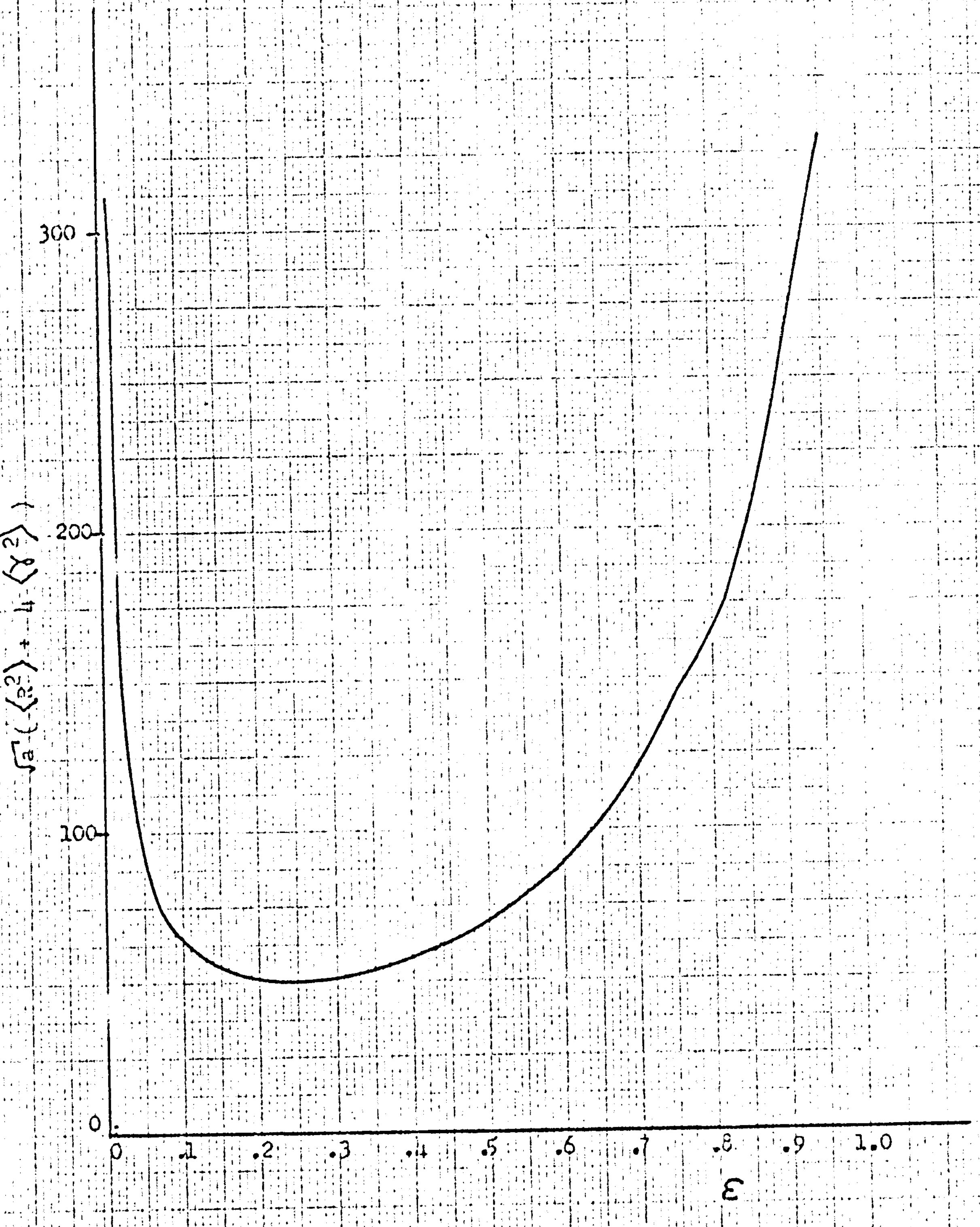

300
200
100
0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.0
ε
$\sqrt{a}\,(\langle \ddot{u}^2 \rangle + 4\langle \gamma^2 \rangle)$

TABLE 4

R.M.S. CLUSTER SEPARATION DATA

ε	$\sqrt{a}\sqrt{\langle R^2\rangle}$	ε	$\sqrt{a}\sqrt{\langle R^2\rangle}$	ε	$\sqrt{a}\sqrt{\langle R^2\rangle}$
.01	5.887	.34	1.145	.68	.796
.02	4.180	.35	1.131	.69	.785
.03	3.427	.36	1.118	.70	.775
.04	2.980	.37	1.106	.71	.765
.05	2.676	.38	1.093	.72	.754
.06	2.452	.39	1.082	.73	.743
.07	2.280	.40	1.070	.74	.732
.08	2.141	.41	1.059	.75	.720
.09	2.027	.42	1.048	.76	.708
.10	1.931	.43	1.037	.77	.696
.11	1.848	.44	1.026	.78	.684
.12	1.777	.45	1.016	.79	.671
.13	1.714	.46	1.006	.80	.657
.14	1.659	.47	.995	.81	.643
.15	1.609	.48	.986	.82	.629
.16	1.565	.49	.976	.83	.614
.17	1.524	.50	.966	.84	.598
.18	1.587	.51	.957	.85	.582
.19	1.454	.52	.947	.86	.564
.20	1.423	.53	.938	.87	.546
.21	1.394	.54	.928	.88	.526
.22	1.367	.55	.919	.89	.506
.23	1.342	.56	.910	.90	.484
.24	1.319	.57	.900	.91	.460
.25	1.297	.58	.891	.92	.434
.26	1.277	.59	.882	.93	.405
.27	1.257	.60	.873	.94	.374
.28	1.239	.61	.863	.95	.338
.29	1.221	.62	.854	.96	.297
.30	1.205	.63	.844	.97	.248
.31	1.189	.64	.835	.98	.183
.32	1.174	.65	.825	.99	.068
.33	1.159	.66	.815	1.00	
		.67	.806		

FIGURE 6

The ground state, expected root mean square separation of the alpha clusters in the Be^8 cluster model as a function of the variational parameters.

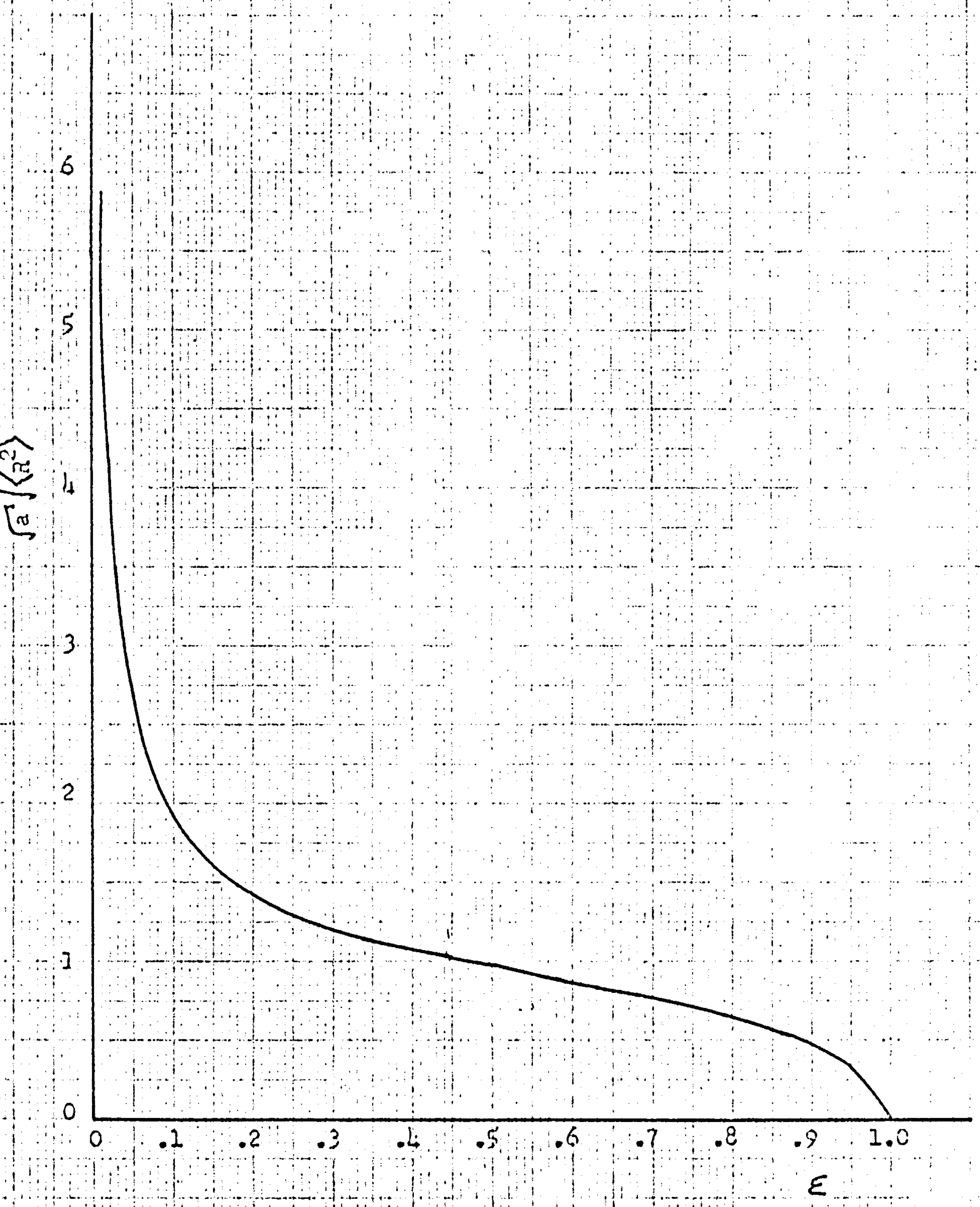

$\sqrt{a}\sqrt{\langle R^2\rangle}$
6
5
4
3
2
1
0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.0
ε

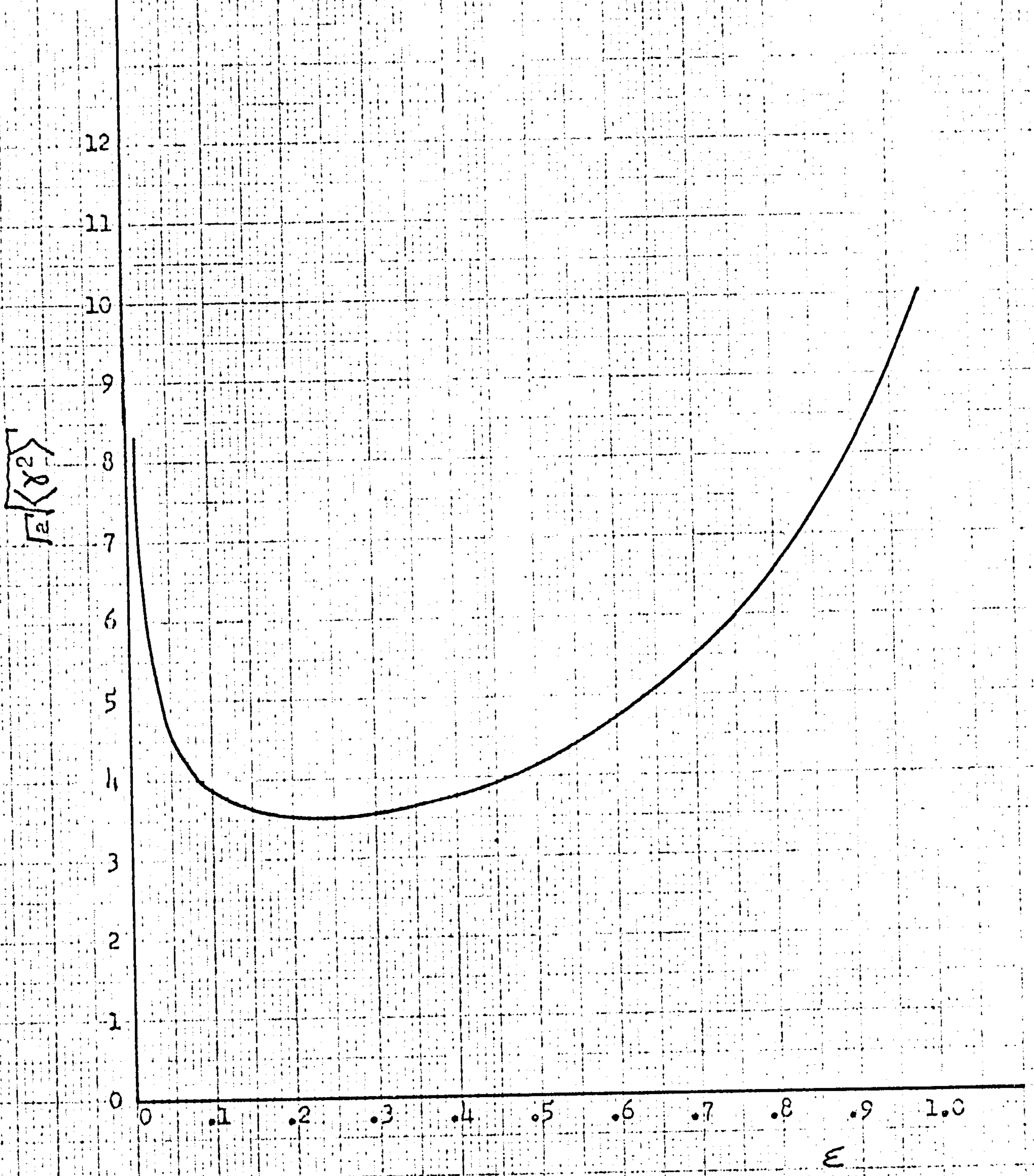
TABLE 5

R.M.S. CLUSTER RADIUS DATA

ε	$\sqrt{\alpha}\sqrt{\langle r^2\rangle}$	ε	$\sqrt{\alpha}\sqrt{\langle r^2\rangle}$	ε	$\sqrt{\alpha}\sqrt{\langle r^2\rangle}$
.01	8.312	.34	3.608	.68	5.321
.02	6.246	.35	3.629	.69	5.409
.03	5.383	.36	3.651	.70	5.500
.04	4.896	.37	3.676	.71	5.594
.05	4.579	.38	3.702	.72	5.691
.06	4.354	.39	3.729	.73	5.791
.07	4.187	.40	3.759	.74	5.894
.08	4.058	.41	3.789	.75	6.000
.09	3.955	.42	3.822	.76	6.111
.10	3.871	.43	3.856	.77	6.224
.11	3.802	.44	3.892	.78	6.342
.12	3.745	.45	3.930	.79	6.463
.13	3.696	.46	3.969	.80	6.589
.14	3.656	.47	4.010	.81	6.718
.15	3.622	.48	4.053	.82	6.852
.16	3.594	.49	4.097	.83	6.991
.17	3.570	.50	4.144	.84	7.134
.18	3.550	.51	4.192	.85	7.282
.19	3.534	.52	4.242	.86	7.436
.20	3.522	.53	4.293	.87	7.595
.21	3.513	.54	4.347	.88	7.759
.22	3.507	.55	4.402	.89	7.929
.23	3.503	.56	4.460	.90	8.106
.24	3.502	.57	4.519	.91	8.289
.25	3.503	.58	4.581	.92	8.478
.26	3.507	.59	4.645	.93	8.675
.27	3.513	.60	4.710	.94	8.878
.28	3.521	.61	4.778	.95	9.090
.29	3.531	.62	4.849	.96	9.309
.30	3.542	.63	4.921	.97	9.537
.31	3.556	.64	4.996	.98	9.774
.32	3.572	.65	5.074	.99	10.020
.33	3.589	.66	5.154	1.00	
		.67	5.236		

FIGURE 7

The ground state, expected root mean square radius of the alpha clusters in the Be^8 cluster model as a function of the variational parameters.



$\Gamma_2 \langle \gamma^2 \rangle$
12
11
10
9
8
7
6
5
4
3
2
1
0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.0
ε

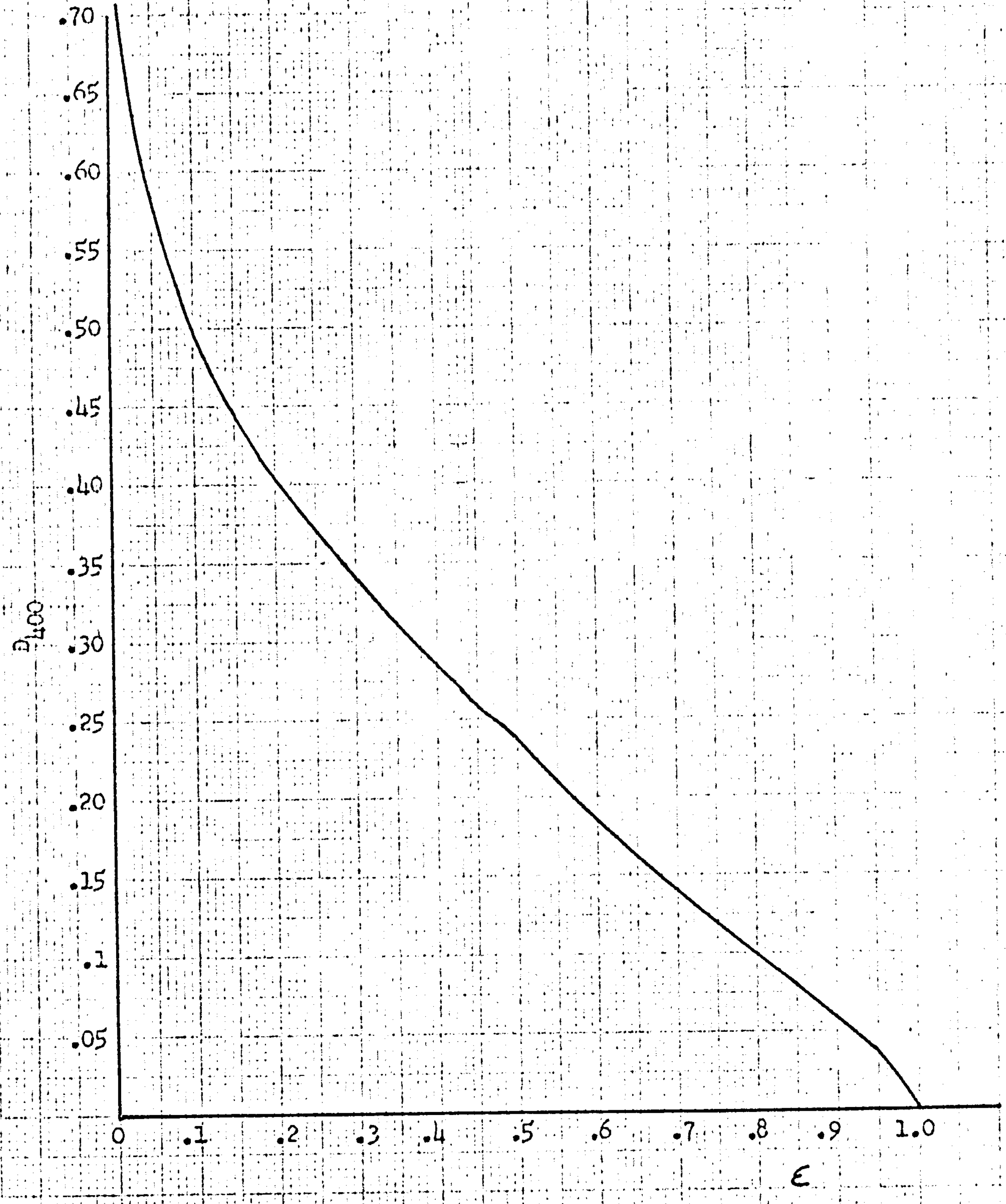
TABLE 6

DUMBBELLEDNESS DATA

.01	.708	.34	.317	.68	.150
.02	.669	.35	.312	.69	.145
.03	.637	.36	.306	.70	.141
.04	.609	.37	.301	.71	.137
.05	.584	.38	.295	.72	.132
.06	.563	.39	.290	.73	.128
.07	.544	.40	.285	.74	.124
.08	.528	.41	.279	.75	.120
.09	.512	.42	.274	.76	.116
.10	.499	.43	.269	.77	.112
.11	.486	.44	.264	.78	.108
.12	.474	.45	.258	.79	.104
.13	.464	.46	.253	.80	.100
.14	.454	.47	.248	.81	.096
.15	.444	.48	.243	.82	.092
.16	.435	.49	.238	.83	.088
.17	.427	.50	.233	.84	.084
.18	.419	.51	.228	.85	.080
.19	.411	.52	.223	.86	.076
.20	.404	.53	.218	.87	.072
.21	.397	.54	.214	.88	.068
.22	.390	.55	.209	.89	.064
.23	.383	.56	.204	.90	.060
.24	.377	.57	.199	.91	.055
.25	.370	.58	.195	.92	.051
.26	.364	.59	.190	.93	.047
.27	.358	.60	.185	.94	.042
.28	.352	.61	.181	.95	.037
.29	.346	.62	.176	.96	.032
.30	.340	.63	.172	.97	.026
.31	.334	.64	.167	.98	.019
.32	.329	.65	.163	.99	.007
.33	.323	.66	.158	1.00	
		.67	.154		

FIGURE 8

The degree of "dumbbelledness" of the nucleus of Be^8 for the ground state according to the cluster model. $D_{N\ell m}$ denotes the degree of clustering of the alpha particles and is defined as the ratio of the expected r.m.s. cluster separation to the expected root mean square radius of the alpha clusters.


a_{400}
.70
.65
.60
.55
.50
.45
.40
.35
.30
.25
.20
.15
.1
.05
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.0
ε

Pearlstein, Tang and Wildermuth (2) have assumed a certain nucleon-nucleon potential(for the details of this potential see reference 2) and found that the values of a and β that correspond to minimized separation energy for the ground state are

$$a = 4.33 \times 10^{25} \quad cm^{-2}$$
$$\beta = 3.15 \times 10^{25} \quad cm^{-2}$$
$$\varepsilon = 0.728$$

From these values and the results obtained in this thesis it follows that for the ground state

$$\sqrt{\langle R^2 \rangle_{400}} = 1.13 \times 10^{-13} \quad cm.$$
$$\sqrt{\langle \gamma^2 \rangle_{400}} = 8.80 \times 10^{-13} \quad cm.$$

Hence from the combined results of the expected alpha cluster radii and expected alpha cluster separation obtained in the work presented here indicate that the cluster model of Wildermuth and Kanellopoulos(Reference 1) with the nucleon-nucleon potential assumed by Pearlstein, Tang, and Wildermuth (Reference 2) predicts that the Be^8 nucleus is ellipsoidal in shape but only very sightly and that the Be^8 nucleus is diffuse.

CONCLUSIONS

In an effort to obtain a physical picture of the cluster model of the Be^8 nucleus, the expected root mean square separation of the clusters, root mean square radius of the alpha clusters, and a quantitative measure of the degree of "dumbbellness" have been obtained as functions of the variational parameters in the cluster model wave functions. The results are given in Figures 2, 3, 5 and6. Employing the values of the parameters obtained in Reference 2 for minimized binding energy it has been found that Be^8 is very slightly ellipsoidal in shape and a very diffuse nucleus.

However, to fully answer the question of whether or not the cluster model describes a collective distortion of the Be^8 wave function,that can be described in shell theory only by including configuration mixing, the cluster radius and separation should be calculated in the shell model. This calculation is now underway along with the considerations of whether or not generalized cluster model wave functions form a complete set.

In this thesis many important mathematical and physical properties of the cluster model have been uncovered. Symmetry considerations of the cluster model have been useful in the development of these mathematical and physical properties.

APPENDIX 1

The object of this appendix is to find the normalization, A_i, in equation (2) on page 5. We have that

$$\phi_{N\ell m} = A_i \exp\left[-\frac{ar^2}{2}\right] r^{\ell}\, L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}}(ar^2)\; Y_{\ell}^{m}(\theta,\phi)$$

The normalization factor, A_i, is determined by the requirement

$$|A_i|^2 \int \exp\left[-ar^2\right] r^{2\ell} \left| L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}}(ar^2)\right|^2 \left| Y_{\ell}^{m}(\theta,\phi)\right|^2 dv = 1$$

where $dv = r^2 \sin\theta\, d\theta d\phi dr$. Hence

$$\left|\frac{1}{A_i}\right|^2 = \int_0^{\pi}\int_0^{2\pi}\int_0^{\infty} \exp\left[-ar^2\right] r^{2\ell} \left| L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}}(ar^2)\right|^2 \left| Y_{\ell}^{m}(\theta,\phi)\right|^2 r^2 \sin\theta d\theta d\phi dr$$

$$= \int_0^{\infty} \exp\left[-ar^2\right] r^{2(\ell+1)} \left| L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}}(ar^2)\right|^2 dr$$

$$= \frac{1}{2a^{\ell+\frac{3}{2}}} \int_0^{\infty} \exp\left[-t\right] t^{\ell+\overset{\ell}{\frac{3}{2}}} \left| L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}}(t)\right|^2 dt \quad (\text{where } t = ar^2)$$

$$= \frac{1}{2a^{\ell+\frac{3}{2}}} \left[\frac{\Gamma(\ell+\frac{3}{2})\,\Gamma(\frac{N+\ell+3}{2})}{\Gamma(\frac{N-\ell}{2}+1)\,\Gamma(\ell+\frac{3}{2})}\right]$$

from the evaluation of the preceding integral in reference (4).

Finally

$$A_i = \left[\frac{2a^{\ell + \frac{3}{2}} \, \Gamma\left(\frac{N-\ell}{2} + 1\right)}{\Gamma\left(\frac{N+}{2} + \frac{3}{2}\right)} \right]^{\frac{1}{2}}$$

APPENDIX 2

The object of this appendix is to prove the identity

$$\sum_{i=1}^{A} r_i^2 = \sum_{j=1}^{k} n_j R_j^2 + \sum_{q=1}^{n_j-1} \gamma_q^{j\,2} + \left(\sum_{q=1}^{n_j-1} \gamma_q^j\right)^2$$

On page 11 it is given that

$$\vec{R}_i = \frac{1}{n_i}\sum_{q=1}^{n_i} \vec{r}_q^{\,i} \text{ and } \vec{\gamma}_1^{\,i} = \vec{r}_1^{\,i} - \vec{R}_i, \ldots\ldots, \vec{\gamma}_{n_i}^{\,i} = \vec{r}_{n_i}^{\,i} - \vec{R}_i$$

Then

$$\sum_{q=1}^{n_i-1}\vec{\gamma}^{\,i}_q = \sum_{q=1}^{n_i-1}\vec{r}^{\,i}_q - (n_i-1)\vec{R}_i = \sum_{q=1}^{n_i}\vec{r}^{\,i}_q - \vec{r}^{\,i}_{n_i} - (n_i-1)\vec{R}_i = -\vec{\gamma}^{\,i}_{n_i}$$

and so

$$\sum_{i=1}^{A} r_i^2 = \sum_{j=1}^{k}\left[\sum_{q=1}^{n_j} r_q^{j\,2}\right] = \sum_{j=1}^{k}\left[\sum_{q=1}^{n_j-1}(\vec{\gamma}^{\,i}_q + \vec{R}_j)^2 + (\vec{R}_j - \sum_{p=1}^{n_j-1}\vec{\gamma}^{\,j}_p)^2\right]$$

$$= \sum_{j=1}^{k}\left[\sum_{q=1}^{n_j-1}(\gamma_q^{j\,2} + 2\,\vec{\gamma}^{\,j}_q\cdot\vec{R}_j + R_j^2) + R_j^2 - 2\vec{R}_j\cdot\sum_{p=1}^{n_j-1}\vec{\gamma}^{\,j}_p + \left(\sum_{p=1}^{n_j-1}\vec{\gamma}^{\,j}_p\right)^2\right]$$

$$= \sum_{j=1}^{k}\left[n_j R_j^2 + \sum_{q=1}^{n_j-1}\gamma_q^{j\,2} + \left(\sum_{q=1}^{n_j-1}\vec{\gamma}^{\,j}_q\right)^2\right]$$

Similarly

$$\sum_{i=1}^{A} \dot{r}_i^2 = \sum_{j=1}^{k}\left[n_j \dot{R}_j^2 + \sum_{q=1}^{n_j-1}\dot{\gamma}_q^{j\,2} + \left(\sum_{q=1}^{n_j-1}\dot{\gamma}^{j}_q\right)^2\right]$$

For simplicity in notation the momenta is written in its classical form, $m\vec{v}$. This, of course, is later replaced by its operator $\frac{\hbar}{i}\vec{\nabla}$ for quantum mechanical calculations.

APPENDIX 3

The purpose of this appendix is to prove the following identities

$$\sum_{i=1}^{3} \gamma_i^2 + \Big(\sum_{i=1}^{3} \gamma_i\Big)^2 = \sum_{i=1}^{3} \beta_i^2$$

and

$$\sum_{j=1}^{2} \left[\frac{P_j^2}{2M_j} + \frac{n_j^2 a^2 \hbar^2}{.2M_j} R_j^2 \right] = \frac{P_{cm}^2}{2M} + \frac{4 n^2 a^2 \hbar^2 R_{cm}^2}{2M} + \frac{P^2}{2\mu} + \frac{1}{4} \frac{n^2 a^2 \hbar^2 R^2}{2\mu}$$

Let:

$$\vec{\beta}^j_1 = \vec{\gamma}^j_2 + \vec{\gamma}^j_3 ; \quad \vec{\beta}^j_2 = \vec{\gamma}^j_3 + \vec{\gamma}^j_1 ; \quad \vec{\beta}^j_3 = \vec{\gamma}^j_1 + \vec{\gamma}^j_2$$

Then it follows that

$$\vec{\gamma}^j_1 = \frac{1}{2} (- \vec{\beta}^j_1 + \vec{\beta}^j_2 + \vec{\beta}^j_3) ; \quad \vec{\gamma}^j_2 = \frac{1}{2} (\vec{\beta}^j_1 - \vec{\beta}^j_2 + \vec{\beta}^j_3) ; \quad \vec{\gamma}^j_3 = \frac{1}{2} (\vec{\beta}^j_1 + \vec{\beta}^j_2 - \vec{\beta}^j_3)$$

and

$${\gamma^j_1}^2 = \frac{1}{4} \left({\beta^j_1}^2 + {\beta^j_2}^2 + {\beta^j_3}^2 - 2\vec{\beta}^j_1 \cdot \vec{\beta}^j_2 - 2\vec{\beta}^j_1 \cdot \vec{\beta}^j_3 + 2\vec{\beta}^j_2 \cdot \vec{\beta}^j_3 \right)$$

$${\gamma^j_2}^2 = \frac{1}{4} \left({\beta^j_1}^2 + {\beta^j_2}^2 + {\beta^j_3}^2 - 2\vec{\beta}^j_1 \cdot \vec{\beta}^j_2 + 2\vec{\beta}^j_1 \cdot \vec{\beta}^j_3 - 2\vec{\beta}^j_2 \cdot \vec{\beta}^j_3 \right)$$

$${\gamma^j_3}^2 = \frac{1}{4} \left({\beta^j_1}^2 + {\beta^j_2}^2 + {\beta^j_3}^2 + 2\vec{\beta}^j_1 \cdot \vec{\beta}^j_2 - 2\vec{\beta}^j_1 \cdot \vec{\beta}^j_3 - 2\vec{\beta}^j_2 \cdot \vec{\beta}^j_3 \right)$$

Therefore

$$\sum_{i=1}^{3} {\gamma^j_i}^2 = \frac{3}{4} \left({\beta^j_1}^2 + {\beta^j_2}^2 + {\beta^j_3}^2 \right) - \frac{1}{2} \left(\vec{\beta}^j_1 \cdot \vec{\beta}^j_2 + \vec{\beta}^j_1 \cdot \vec{\beta}^j_3 + \vec{\beta}^j_2 \cdot \vec{\beta}^j_3 \right)$$

Also

$$\sum_{i=1}^{3} \vec{\gamma}_i^{\,j} = \frac{1}{2}\sum_{i=1}^{3} \vec{\beta}_i \text{ and so } \Big(\sum_{i=1}^{3} \gamma_i^{j}\Big)^2 = \frac{1}{4}\Big(\beta_1^{j\,2} + \beta_2^{j\,2} + \beta_3^{j\,3} + 2\vec{\beta}_1^{\,j}\cdot\vec{\beta}_2^{\,j} + \vec{\beta}_1^{\,j}\cdot\vec{\beta}_3^{\,j} + \vec{\beta}_2^{\,j}\cdot\vec{\beta}_3^{\,j}\Big)$$

Therefore

$$\sum_{i=1}^{3} \gamma_i^{j\,2} + \Big(\sum_{i=1}^{3} \gamma_i^{j}\Big)^2 = \sum_{i=1}^{3} \beta_i^{j\,2} \text{ and similarly } \sum_{i=1}^{3} \dot{\gamma}_i^{j\,2} + \Big(\sum_{i=1}^{3} \dot{\gamma}_i^{j}\Big)^2 = \sum_{i=1}^{3} \dot{\beta}_i^{j\,2}$$

This proves the first identity. Consider the second identity: Define $\vec{R}$ and $\vec{R}_{cm}$ as follows:

$$\vec{R} = \vec{R}_1 - \vec{R}_2; \quad \vec{R}_{cm} = \frac{\vec{R}_1 + \vec{R}_2}{2}$$

Thus

$$\vec{R}_1 = \frac{\vec{R}}{2} + \vec{R}_{cm}; \quad \vec{R}_2 = \vec{R}_{cm} - \frac{\vec{R}}{2}$$

and

$$R_1^2 = R_{cm}^2 + \vec{R}\cdot\vec{R}_{cm} + \frac{R^2}{4}; \quad R_2^2 = R_{cm}^2 - \vec{R}\cdot\vec{R}_{cm} + \frac{R^2}{4}$$

Therefore

$$R_1^2 + R_2^2 = 2R_{cm}^2 + \frac{R^2}{2} \text{ and similarly, } \dot{R}_1^2 + \dot{R}_2^2 = 2\dot{R}_{cm}^2 + \frac{\dot{R}^2}{2}$$

Then

$$P_1^2 + P_2^2 = (4m\dot{R}_1)^2 + (4m\dot{R}_2)^2 = 32m^2\,\dot{R}_{cm}^2 + 8m^2\,\dot{R}^2$$

and

$$\sum_{j=1}^{2}\left[\frac{P_j^2}{2M_j} + \frac{n_j^2 a^2 \hbar^2 R_j^2}{2M_j}\right] = \frac{1}{8m}\left[32m^2\,R_{cm}^2 + 8m^2\,R^2 + 2n^2a^2\hbar^2\,R_{cm}^2 + \frac{n^2a^2\hbar^2\,R^2}{2}\right]$$

$$= \frac{(8mR_{cm})^2}{2M} + \frac{(2mR)^2}{2\mu} + \frac{4n^2a^2\hbar^2R_{cm}^2}{2M} + \frac{n^2a^2\hbar^2}{4}\,\frac{R^2}{2\mu}$$

$$= \frac{P_{cm}^2}{2M} + \frac{4n^2a^2\hbar^2\,R^2{}_{cm}}{2M} + \frac{P^2}{2\mu} + \frac{1}{4}\,\frac{n^2a^2\hbar^2\,R^2}{2\mu}$$

APPENDIX 4

In this appendix it is shown that the function,

$$\exp\left[-\frac{a}{2}\sum_{i=1}^{6}\beta_i^2\right]\exp\left[-\frac{2aR^2}{2},\right]$$

is symmetric with respect to an interchange of any two position vectors, $\vec{r}_i$ and $\vec{r}_j$.

The problem at hand is, essentially, to show that $\sum_{i=1}^{6}\beta_i^2 + 2R^2$ is invariant with respect to an interchange of any two position vectors, $\vec{r}_i$ and $\vec{r}_j$. It follows from Appendices 2 and 3 that

$$\sum_{i=1}^{6}\beta_i^2 = \sum_{i=1}^{8}\gamma_i^2$$

Also from equation (8), on page 11 it follows that

$$\gamma_i^{j\,2} = r_i^{j\,2} - 2\vec{R}_j\cdot\vec{r}_i^{\,j} + R_j^2 \quad \text{and} \quad \sum_{i=1}^{4}\gamma_i^{j\,2} = \sum_{i=1}^{4}r_i^{j\,2} - 2\vec{R}_j\cdot\sum_{i=1}^{4}\vec{r}_i^{\,j} + 4R_j^2$$

Therefore

$$\sum_{i=1}^{8}\gamma_i^2 = \sum_{j=1}^{2}\sum_{i=1}^{4}\gamma_i^{j\,2} = \sum_{i=1}^{8}r_i^2 - 4(R_1^2 + R_2^2)$$

Also

$$2R^2 = 2(R_1-R_2)^2 = 2(R_1^2 - 2\vec{R}_1\cdot\vec{R}_2 + R_2^2)$$

This finally gives

$$\sum_{i=1}^{6}\beta_i^2 + 2R^2 = \sum_{i=1}^{8}r_i^2 - 2(\vec{R}_1+\vec{R}_2)^2 = \sum_{i=1}^{8}r_i^2 - \frac{1}{8}\left(\sum_{i=1}^{8}\vec{r}_i\right)^2$$

which is seen to be invariant with respect to an interchange of any two position vectors, $\vec{r}_i$ and $\vec{r}_j$.

APPENDIX 5

It will be shown here that the spatial antisymmetrization of the function $f(R) = -10\,aR^2 + \frac{15}{4}$, with respect to an interchange of any two position vectors yields a zero result, i.e.

$$\mathcal{A}_s \left(-10aR^2 + \frac{15}{4} \right) = 0$$

where $\mathcal{A}_s$ denotes a spatial antisymmetrization operator.

It has been seen, in the formulation of the cluster model, that the model is often "stabilized" into the realm of the independent particle model. This stabilization process is a consistent feature in the construction of the cluster model. This "principle of stabilization" will now be applied in the following antisymmetrization process.

From equation (2), page 5, we have the result that the single independent particle wave functions are given by

$$\phi_i = A_i \exp\left[-\frac{ar^2}{2} \right] r^{\ell} L_{\frac{N-\ell}{2}}^{\ell+\frac{1}{2}} (ar^2)\, Y_{\ell}^{m} (\theta, \phi)$$

where

$$A_i = \left[\frac{2a^{\ell+\frac{3}{2}}\,\Gamma\left(\frac{N-\ell}{2}+1\right)}{\Gamma\left(\frac{N+\ell+1}{2}\right)} \right]^{\frac{1}{2}}$$

It follows from this that the single particle S-state wave function is given by

$$S = \left[\frac{a}{\pi}\right]^{\frac{3}{2}} \exp\left[-\frac{ar^2}{2} \right] = \left[\frac{a}{\pi}\right]^{\frac{3}{2}} \exp\left[-\frac{ar^2}{2} \right] s:(N,\ell,m) = (0,0,0)$$

In the 1P state the single particle wave functions are

$$P_{10} = \left[\frac{2a^{\frac{5}{2}}}{\pi^{\frac{3}{2}}}\right]^{\frac{1}{2}} \exp\left[-\frac{ar^2}{2}\right] z : (N,\ell,m) = (1,1,0)$$

$$P_{11} = -\left[\frac{a^{\frac{5}{2}}}{\pi^{\frac{3}{2}}}\right]^{\frac{1}{2}} \exp\left[-\frac{ar^2}{2}\right](x+iy) : (N,\ell,m) = (1,1,1)$$

$$P_{1-1} = \left[\frac{a^{\frac{5}{2}}}{\pi^{\frac{3}{2}}}\right]^{\frac{1}{2}} \exp\left[-\frac{ar^2}{2}\right](x-iy) : (N,\ell,m) = (1,1,-1)$$

where $z = r\cos\phi$, $y = r\sin\phi$, and $x = r\sin\theta\cos\phi$ and $s=1$ To simplify the notation we can let,

$$s = 1,\quad a = z,\quad b = x + iy,\quad \text{and } c = x - iy$$

Also

$$\vec{R} = \vec{R}_{12} = \frac{\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4 - \vec{r}_5 - \vec{r}_6 - \vec{r}_7 - \vec{r}_8}{4}$$

$$= \left(\frac{x_1 + x_2 + x_3 + x_4 - x_5 - x_6 - x_7 - x_8}{4}\right)\vec{i}_1$$

$$+ \left(\frac{y_1 + y_2 + y_3 + y_4 - y_5 - y_6 - y_7 - y_8}{4}\right)\vec{i}_2$$

$$+ \left(\frac{z_1 + z_2 + z_3 + z_4 - z_5 - z_6 - z_7 - z_8}{4}\right)\vec{i}_3$$

where the subscripts denote the associated particle. With the above notation we have,

$$z = a, \; x = \frac{b + c}{2}, \text{ and } y = \frac{b - c}{2i}$$

With this the expression for R_{12} becomes

$$\vec{R}_{12} = \left(\frac{b_{12} + c_{12}}{2}\right)\vec{i}_1 + \left(\frac{b_{12} - c_{12}}{2i}\right)\vec{i}_2 + a_{12}\,\vec{i}_3$$

where

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

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

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

It now follows that

$$R_{12}^2 = a_{12}^2 + b_{12}c_{12}$$

and

$$\mathcal{A}R^2 = \mathcal{A}R_{12}^2 = \mathcal{A}a_{12}^2 + \mathcal{A}b_{12}c_{12}$$

Consider the term

$$a_{12}^2 = \frac{1}{4^2}\left[a_1 + a_2 + a_3 + a_4 - a_5 - a_6 - a_7 - a_8\right]^2$$

In the frame of the independent particle model each term in the expression for R^2 should be a product of all eight single particle wave functions. When the above expression is multiplied out only the linear terms are kept since the a_i^2 terms do not correspond to a product of

Table XIX.-

Inter-Variable Correlation Coefficients

	Age	Faculty	Ststat	Presemp	Marstat	Edcomp	Nyrsch	Birthpl	Fbirth	Mbirth
Age	1.000									
Faculty	-0.109	1.000								
Ststat	0.458	0.020	1.000							
Presemp	-0.429	-0.037	-0.693	1.000						
Marstat	0.408	-0.087	0.371	-0.236	1.000					
Edcomp	-0.088	0.001	-0.133	0.107	-0.021	1.000				
Nyrsch	0.208	0.048	-0.031	-0.007	0.151	0.571	1.000			
Birthpl	0.054	-0.049	-0.001	-0.168	0.052	0.031	0.050	1.000		
Fbirth	99.000	99.000	99.000	99.000	99.000	99.000	99.000	99.000	99.000	
Mbirth	99.000	99.000	99.000	99.000	99.000	99.000	99.000	99.000	99.000	99.000
Rsdence	0.032	-0.127	-0.019	-0.059	-0.020	-0.104	-0.141	-0.040	99.000	99.000
Populatn	0.091	-0.162	0.136	-0.181	0.066	-0.191	-0.217	-0.050	99.000	99.000
Local	0.016	0.052	-0.040	-0.125	-0.044	0.118	0.107	0.756	99.000	99.000

*Note: A value of 99.000 was printed if a coefficient could not be computed

APPENDIX 3

Table XIX.-

Inter-Variable Correlation Coefficients

	Age	Faculty	Ststat	Presemp	Marstat	Edcomp	Nyrsch	Birthpl	Fbirth	Mbirth
Nbros	0.066	0.049	-0.008	-0.071	0.007	-0.052	-0.119	-0.018	99.000	99.000
Noldbros	-0.088	0.077	0.002	-0.009	-0.052	0.026	-0.043	-0.022	99.000	99.000
Nsis	-0.011	-0.028	0.071	-0.077	0.017	0.021	0.014	-0.055	99.000	99.000
Noldsis	-0.001	0.139	0.134	-0.106	0.003	0.009	0.009	-0.028	99.000	99.000
Birthord	-0.122	0.173	0.019	0.007	-0.054	-0.008	-0.054	-0.052	99.000	99.000
Fedcomp	-0.127	0.036	-0.079	0.103	0.037	-0.032	0.018	0.028	99.000	99.000
Medcomp	-0.013	-0.067	0.005	-0.032	-0.001	-0.082	0.012	0.123	99.000	99.000
Fathemp	-0.101	0.051	-0.093	0.132	0.008	-0.094	0.013	0.005	99.000	99.000
Religion	-0.014	-0.125	-0.003	-0.020	0.076	-0.037	0.161	0.120	99.000	99.000
Cmtong	-0.051	0.077	-0.068	0.008	-0.137	0.175	0.036	-0.196	99.000	99.000
Fmtong	-0.051	0.077	-0.068	0.008	-0.137	0.175	0.036	-0.196	99.000	99.000
Mmtong	-0.051	0.077	-0.068	0.008	-0.137	0.175	0.036	-0.196	99.000	99.000
Homeperc	0.098	-0.012	0.040	-0.031	0.110	-0.031	0.020	-0.006	99.000	99.000
Outperc	0.075	0.051	0.013	-0.033	0.056	-0.022	0.058	-0.048	99.000	99.000

*Note: A value of 99.000 was printed if a coefficient could not be computed

APPENDIX 7

The purpose of this appendix is to prove the following identity:

$$\int \mathcal{S} f(\vec{x}_1 \ldots \vec{x}_N) \; d\vec{x}_1 \ldots d\vec{x}_N = \sqrt{N!} \int f(\vec{x}_1 \ldots \vec{x}_N) \; d\vec{x}_1 \ldots d\vec{x}_N$$

where $\mathcal{S}$ is the symmetrization operator and $f(\vec{x}_1 \ldots \vec{x}_N)$ is some function of the N independent variables, $\vec{x}_i$.

It is clear that

$$\mathcal{S} f(\vec{x}_1 \ldots \vec{x}_N) = \frac{1}{\sqrt{N!}} \int f(\vec{x}'_1 \ldots \vec{x}'_N) \begin{bmatrix} \delta(\vec{x}_1-\vec{x}'_1) \ldots\ldots\ldots \delta(\vec{x}_1-\vec{x}'_N) \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \delta(\vec{x}_N-\vec{x}'_1) \ldots\ldots\ldots \delta(\vec{x}_N-\vec{x}'_N) \end{bmatrix} d\vec{x}'_1 \ldots d\vec{x}'_N$$

where $\begin{bmatrix} \ldots \end{bmatrix}$ denotes a permanent; that is, a determinant expanded in the normal way except that all the terms are added and there is never any subtraction involved. Hence

$$\int \mathcal{S} f(\vec{x}_1 \ldots \vec{x}_N) \; d\vec{x}_1 \ldots d\vec{x}_N = \frac{1}{\sqrt{N!}} \iint f(\vec{x}'_1 \ldots \vec{x}'_N) \begin{bmatrix} \delta(\vec{x}_1-\vec{x}'_1) \ldots \delta(\vec{x}_1-\vec{x}'_N) \\ \delta(\vec{x}_N-\vec{x}'_1) \ldots \delta(\vec{x}_N-\vec{x}'_N) \end{bmatrix} d\vec{x}_1 \ldots d\vec{x}_N \, d\vec{x}'_1 \cdot d\vec{x}'_N$$

$$= \frac{1}{\sqrt{N!}} \int f(\vec{x}'_1 \ldots \vec{x}'_N) \; N! \; d\vec{x}'_1 \ldots d\vec{x}'_N$$

(after integrating over the unprimed system.)

$$= \sqrt{N!} \int f(\vec{x}_1 \ldots \vec{x}_N) \; d\vec{x}_1 \ldots d\vec{x}_N$$

APPENDIX 8

In this appendix a summation over the intrinsic and isotopic spin coordinates in equation (25) page 29 is performed.

Equation (25) is of the following form:

$$D\alpha\sqrt{24!}\int\left[\mathcal{A}\; G_{N\ell m}X(S,T)\right]^{*} P\left[\delta(\vec{r}_1-\vec{r}\,'_1)\dots\,\delta(t_8,-\frac{1}{2})\right] G_{N\ell m}X(S,T)\; d\tau$$

This can be written

$$D\alpha\iint G_{N\ell m}(\,..\vec{r}\,''_i..\,)X(S,T)''\begin{vmatrix} \delta(\vec{r}_1-\vec{r}\,''_1)\,\delta(s_1,s''_1)\,\delta(t_1,t''_1)\,..\,\delta(\vec{r}_1-\vec{r}\,''_8)\delta(s_1,s''_8)\;\delta(t_1-t''_8) \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\ \delta(\vec{r}_8-\vec{r}\,''_1)\,\delta(s_8,s''_1)\delta(t_8,t''_1)\,..\,\delta(\vec{r}_8-\vec{r}\,''_8)\;\delta(s_8,s''_8)\;\delta(t_8,t''_8) \end{vmatrix} d$$

$$\begin{bmatrix} \delta(\vec{r}_1-\vec{r}\,'_1)\;\delta(s_1,s'_1)\;\delta(t_1,t'_1)\dots\delta(\vec{r}_1-\vec{r}\,'_8)\;\delta(s_1,s'_8)\;\delta(t_1,t'_8) \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\ \delta(\vec{r}_8-\vec{r}\,'_1)\;\delta(s_8,s'_1)\;\delta(t_8,t'_1)\dots\delta(\vec{r}_8-\vec{r}\,'_8)\;\delta(s_8,s'_8)\;\delta(t_8,t'_8) \end{bmatrix} G_{N\ell m}(\,..\vec{r}_i.\,)X(S,T)d$$

where

$$X(S,T) = \delta(s_1,\frac{1}{2})\;\delta(t_1,\frac{1}{2})\;\delta(s_2,\frac{1}{2})\;\delta(t_2,-\frac{1}{2})\;\delta(s_3,-\frac{1}{2})\;\delta(t_3,\frac{1}{2})\;\delta(s_4,-\frac{1}{2})\;\delta(t_4,-\frac{1}{2})$$

$$\delta(s_5,\frac{1}{2})\;\delta(t_5,\frac{1}{2})\;\delta(s_6,\frac{1}{2})\;\delta(t_6,-\frac{1}{2})\;\delta(s_7,-\frac{1}{2})\;\delta(t_7,\frac{1}{2})\;\delta(s_8,-\frac{1}{2})\;\delta(t_8,-\frac{1}{2})$$

$$X(S,T)'' = \delta(s_1,s''_1)\,\delta(t_1,t''_1)\,\delta(s_2,s''_2)\,\delta(t_2,t''_2)\dots\dots\delta(t_7,t''_7)\;\delta(s_8,s''_8)\,\delta(t_8,t''_8)$$

The above integral signs include summations over the unprimed and primed intrinsic and isotopic spin coordinates. Performing this summation assigns the following specific values to s''_i, t''_i, s_i, and t_i:

$s_1'' = s_1 = \frac{1}{2},\ t_1'' = t_1 = \frac{1}{2},\ s_2'' = s_2 = \frac{1}{2}, \ldots . s_8'' = s_8 = -\frac{1}{2},\ t_8'' = t_8 = -\frac{1}{2}$

Therefore

$$D\alpha \iint G_{N\ell m} \ (\ldots \vec{r}_1'' \ldots)^*$$

$$\begin{vmatrix}
\delta(\vec{r}_1-\vec{r}_1'') & 0 & 0 & 0 & \delta(\vec{r}_1-\vec{r}_5'') & 0 & 0 & 0 \\
0 & \delta(\vec{r}_2-\vec{r}_2'') & 0 & 0 & 0 & \delta(\vec{r}_2-\vec{r}_6'') & 0 & 0 \\
0 & 0 & \delta(\vec{r}_3-\vec{r}_3'') & 0 & 0 & 0 & \delta(\vec{r}_3-\vec{r}_7'') & 0 \\
0 & 0 & 0 & \delta(\vec{r}_4-\vec{r}_4'') & 0 & 0 & 0 & \delta(\vec{r}_4-\vec{r}_8'') \\
\delta(\vec{r}_5-\vec{r}_1'') & 0 & 0 & 0 & \delta(\vec{r}_5-\vec{r}_5'') & 0 & 0 & 0 \\
0 & \delta(\vec{r}_6-\vec{r}_2'') & 0 & 0 & 0 & \delta(\vec{r}_6-\vec{r}_6'') & 0 & 0 \\
0 & 0 & \delta(\vec{r}_7-\vec{r}_3'') & 0 & 0 & 0 & \delta(\vec{r}_7-\vec{r}_7'') & 0 \\
0 & 0 & 0 & \delta(\vec{r}_8-\vec{r}_4'') & 0 & 0 & 0 & \delta(\vec{r}_8-\vec{r}_8'')
\end{vmatrix}$$

$$d\tau'' G_{N\ell m} \ (\ldots \vec{r}_i \ldots)$$

$$\begin{bmatrix}
\delta(\vec{r}_1-\vec{r}_1') & 0 & 0 & 0 & \delta(\vec{r}_1-\vec{r}_5') & 0 & 0 & 0 \\
0 & \delta(\vec{r}_2-\vec{r}_2') & 0 & 0 & 0 & \delta(\vec{r}_2-\vec{r}_6') & 0 & 0 \\
0 & 0 & \delta(\vec{r}_3-\vec{r}_3') & 0 & 0 & 0 & \delta(\vec{r}_3-\vec{r}_7') & 0 \\
0 & 0 & 0 & \delta(\vec{r}_4-\vec{r}_4') & 0 & 0 & 0 & (\vec{r}_3-\vec{r}_8') \\
\delta(\vec{r}_5-\vec{r}_1') & 0 & 0 & 0 & \delta(\vec{r}_5-\vec{r}_5') & 0 & 0 & 0 \\
0 & \delta(\vec{r}_6-\vec{r}_2') & 0 & 0 & 0 & \delta(\vec{r}_6-\vec{r}_6') & 0 & 0 \\
0 & 0 & \delta(\vec{r}_7-\vec{r}_3') & 0 & 0 & 0 & \delta(\vec{r}_7-\vec{r}_7') & 0 \\
0 & 0 & 0 & \delta(\vec{r}_8-\vec{r}_4') & 0 & 0 & 0 & \delta(\vec{r}_8-\vec{r}_8')
\end{bmatrix} d\tau$$

where the integration signs no longer include summations over the spin and charge coordinates. A tedious expansion of the above determinant yields the identity,

$$\begin{vmatrix} \delta(\vec{r}_1-\vec{r}_1^{\,\prime\prime}) & \ldots\ldots\ldots & 0 \\ 0 & \ldots\ldots\ldots & 0 \\ 0 & \ldots\ldots\ldots & 0 \\ 0 & \ldots\ldots\ldots & \delta(\vec{r}_4-\vec{r}_8^{\,\prime\prime}) \\ \delta(\vec{r}_5-\vec{r}_1^{\,\prime\prime}) & \ldots\ldots\ldots & 0 \\ 0 & \ldots\ldots\ldots & 0 \\ 0 & \ldots\ldots\ldots & 0 \\ 0 & \ldots\ldots\ldots & \delta(\vec{r}_8-\vec{r}_8^{\,\prime\prime}) \end{vmatrix} = (P_{48}-1)(P_{37}-1)(P_{26}-1)(P_{15}-1)\,\delta(\vec{r}_1-\vec{r}_1^{\,\prime\prime}) \times \delta(\vec{r}_2-\vec{r}_2^{\,\prime\prime})\ldots\ldots\;\delta(\vec{r}_8-\vec{r}_8^{\,\prime\prime})$$

where P_{ij} is a spatial exchange operator. It interchanges $\vec{r}_i$ and $\vec{r}_j$.

It now follows that

$$\begin{bmatrix} \delta(\vec{r}_1-\vec{r}_1^{\,\prime}) & \ldots\ldots & 0 \\ 0 & \ldots\ldots & 0 \\ 0 & \ldots\ldots & 0 \\ 0 & \ldots\ldots & \delta(\vec{r}_4-\vec{r}_8^{\,\prime}) \\ \delta(\vec{r}_5-\vec{r}_1^{\,\prime}) & \ldots\ldots & 0 \\ 0 & \ldots\ldots & 0 \\ 0 & \ldots\ldots & 0 \\ 0 & \ldots\ldots & \delta(\vec{r}_8-\vec{r}_8^{\,\prime}) \end{bmatrix} = (P_{48}+1)(P_{37}+1)(P_{26}+1)(P_{15}+1)\;\delta(r_1-r_1')\,\delta(r_2-r_2')\ldots\;\delta(r_8-r_8')$$

But,

$$(P_{48}-1)(P_{37}-1)(P_{26}-1)(P_{15}-1) = 2(1-P_{26}-P_{15}-P_{37}-P_{48} + P_{48}P_{37} + P_{26}P_{37})$$

and

$$(P_{48}+1)(P_{37}+1)(P_{26}+1)(P_{15}+1) = 2(1+P_{26}+P_{15}+P_{37}+P_{48}+P_{48}P_{37}+P_{26}P_{37})$$

Therefore an integration over the double primed system of coordinates gives the following result:

$$D\alpha \int' \Big[\overset{*}{G}_{N\ell m} - P_{26}\overset{*}{G}_{N\ell m} - P_{15}\overset{*}{G}_{N\ell m} - P_{37}\overset{*}{G}_{N\ell m} - P_{48}\overset{*}{G}_{N\ell m} + P_{48}P_{37}\overset{*}{G}_{N\ell m} + P_{37}P_{26}\overset{*}{G}_{N\ell m} + P_{48}P_{26}\overset{*}{G}_{N\ell m} \Big] G_{N\ell m}(1+P_{26}+P_{15}+P_{37}+P_{48}+P_{48}P_{37} + P_{37}P_{26}+P_{48}P_{26})\ \delta(\vec{r}_1-\vec{r}\,'_1)\ \delta(\vec{r}_2-\vec{r}\,'_2)\ \delta(\vec{r}_3-\vec{r}\,'_3)\ \delta(\vec{r}_4-\vec{r}\,'_4)\ \delta(\vec{r}_5-\vec{r}\,'_5)\ \delta(\vec{r}_6-\vec{r}\,'_6)\ \delta(\vec{r}_7-\vec{r}\,'_7)\ \delta(\vec{r}_8-\vec{r}\,'_8)\ d\tau$$

APPENDIX 3

Table XIX.-

Inter-Variable Correlation Coefficients

	Ethaff	Fullemp	Majinf	Famunit	Chstat	Famdisc	Pardisc	Nyrslang	Chcont	Adolcont	Sex
Ethaff	1.000										
Fullemp	0.070	1.000									
Majinf	0.151	-0.094	1.000								
Famunit	0.137	-0.052	0.102	1.000							
Chstat	0.195	-0.019	0.016	0.016	1.000						
Famdisc	0.132	0.060	-0.004	-0.198	0.096	1.000					
Pardisc	-0.029	-0.006	-0.074	0.025	-0.097	0.081	1.000				
Nyrslang	-0.010	0.013	0.052	0.108	-0.023	0.040	0.020	1.000			
Chcont	0.021	-0.030	0.049	-0.040	0.096	0.094	-0.002	-0.083	1.000		
Adolcont	-0.282	-0.024	-0.058	-0.072	-0.033	-0.050	0.032	-0.151	0.465	1.000	
Sex	-0.116	0.024	-0.098	-0.168	0.088	0.007	0.050	0.150	0.102	0.075	1.000

$$
\begin{aligned}
+\ 2\,\mathrm{Re}\Big[& -\psi(o)^{*}\psi(26)-\psi(o)^{*}\psi(15)-\psi(o)^{*}\psi(37)-\psi(o)^{*}\psi(48)+\psi(o)^{*}\psi(48,37) \\
& +\psi(o)^{*}\psi(37,26)+\psi(o)^{*}\psi(48,26)-\psi(15)^{*}\psi(37,48)-\psi(15)^{*}\psi(26,48) \\
& -\psi(15)^{*}\psi(15,48)+\psi(15)^{*}\psi(37)-\psi(26)^{*}\psi(37,48)-\psi(26)^{*}\psi(26,37) \\
& -\psi(26)^{*}\psi(48,26)+\psi(26)^{*}\psi(15)+\psi(26)^{*}\psi(37)+\psi(26)^{*}\psi(48)-\psi(37)^{*}\psi(26,3 \\
& -\psi(37)^{*}\psi(15,37)-\psi(37)^{*}\psi(37,48)+\psi(37)^{*}\psi(48)-\psi(48)^{*}\psi(26,48) \\
& -\psi(48)^{*}\psi(15,48)-\psi(48)^{*}\psi(37,48)+\psi(48,37)^{*}\psi(26,48)+\psi(48,37)^{*} \\
& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\psi(26,37 \\
& +\psi(37,26)^{*}\psi(26,48)+\psi(15)^{*}\psi(48)\Big]
\end{aligned}
$$

APPENDIX 10

In this appendix it is shown that the determinant at the bottom of page 37 satisfies the following identity (at least for the calculation of the expectation value of dynamical quantities).

$$\begin{vmatrix} \delta(\vec{r}_1-\vec{r}\,'_1) & \cdots\cdots\cdots & 0 \\ 0 & \cdots\cdots\cdots & 0 \\ 0 & \cdots\cdots\cdots & 0 \\ 0 & \cdots\cdots\cdots & \delta(\vec{r}_4-\vec{r}\,'_8) \\ \delta(\vec{r}_5-\vec{r}\,'_1) & \cdots\cdots\cdots & 0 \\ 0 & \cdots\cdots\cdots & 0 \\ 0 & \cdots\cdots\cdots & 0 \\ 0 & \cdots\cdots\cdots & \delta(\vec{r}_8-\vec{r}\,'_8) \end{vmatrix} = 2(1-4P_{48}+3P_{37}P_{48})\ \delta(\vec{r}_1-\vec{r}\,'_1)\,.\,.\ \delta(\vec{r}_8-\vec{r}\,'_8)$$

In Appendix 8 it was stated that the above determinant is equal to $(P_{48}-1)(P_{37}-1)(P_{26}-1)(P_{15}-1)\,\delta(\vec{r}_1-\vec{r}\,'_1)\,.\,.\,.\,.\,.\ \delta(\vec{r}_8-\vec{r}\,'_8)$. Hence it remains to be shown that:

$$(P_{48}-1)(P_{37}-1)(P_{26}-1)(P_{15}-1) = 2(1-4P_{48}+3P_{37}P_{48})$$

Now,

$$(P_{48}-1)(P_{37}-1)(P_{26}-1)(P_{15}-1)=P_{48}P_{37}P_{26}P_{15}-P_{48}P_{37}P_{26}-P_{48}P_{37}P_{4}$$

$$-P_{37}P_{26}P_{15}+P_{48}P_{37}+P_{48}P_{15}+P_{48}P_{26}+P_{37}P_{15}+P_{37}P_{26}+P_{26}P_{15}$$

$$-P_{48}-P_{37}-P_{15}-P_{26}+1$$

From the symmetry of the system it follows that:

$P_{48}P_{37}P_{26}P_{15} = 1$, $P_{48}P_{37}P_{15} = P_{26}$, $P_{48}P_{37}P_{26}=P_{15}$,

$P_{37}P_{26}P_{15} = P_{48}$; $P_{48}P_{37}= P_{26}P_{15}$, $P_{48}P_{15}=P_{26}P_{37}$, $P_{48}P_{26}=P_{15}P_{37}$

for the cluster model wave function in the ground state and first two excited states. These equivalence relationships between the exchange operators can be seen as follows

$$P_{15}P_{26}\vec{R} = -P_{37}P_{48}\vec{R} = P P_{26}P_{15}\vec{R}$$

where the P void of subscripts is the parity operator.

Similarly

$$P_{15}P_{26}P_{37}\vec{R} = -P_{48}\vec{R} = P P_{48}\vec{R}$$

Now, consider the nuclear wave function

$$\psi(o) = \exp\left[-\tfrac{1}{2}a\sum_{i=1}^{8}\gamma_i^2\right] R^4 \exp\left[-\beta R^2\right] Y_\ell^m(\Omega)$$

From the last paragraph it is seen that the equivalence relations are strictly true when the operators are operating on R^4 and $\exp\left[-\beta R^2\right]$. Also writing $\gamma_1^2 = (\vec{r}_1 - \vec{R}_1)^2$, ... $\gamma_8^2 = (\vec{r}_8 - \vec{R}_2)^2$ it is seen that the given equivalence relations are valid with respect to the function $\exp\left[-\tfrac{1}{2}a\sum_{i=1}^{8}\gamma_i^2\right]$.

However it is seen that

$$P_{48}P_{37}Y_\ell^m(\Omega) = P_{26}P_{15}\,P\,Y_\ell^m(\Omega)$$

and

$$P_{48}P_{37}P_{26}Y_\ell^m(\Omega) = P_{15}\,P\,Y_\ell^m(\Omega)$$

The parity operation with respect to spherical harmonic functions given by

$$P\,Y_\ell^m(\Omega) = (-1)^\ell\,Y_\ell^m(\Omega)$$

Since $\ell=0,2,4$ in the three lowest states the equivalences are true.

Therefore,

$$(P_{48}-1)(P_{37}-1)(P_{26}-1)(P_{15}-1)=2(1-P_{26}-P_{15}-P_{37}-P_{48}+P_{48}P_{37}$$

$$+P_{37}P_{26}+P_{48}P_{26})$$

Furthermore, it is seen from Appendix 12 that P_{26}, P_{15}, P_{37}, and P_{48}, will each produce exactly the same effect in the calculation of the expectation values. Hence the identity holds for calculations of expectation values.

APPENDIX 11

In this appendix the following identity is proved,

$$\int \psi^*_{N\ell m}\, \mathcal{O}\, \psi_{N\ell m}\, d\tau = \iint G_{N\ell m}(\,.\vec{r}_i^{\,\prime}..\,)^*\, X(S,T)'$$

$$\begin{vmatrix} \delta(\vec{r}_1-\vec{r}_1^{\,\prime})\ \delta(s_1,s_1')\ \delta(t_1,t_1')\ ..\ \delta(\vec{r}_1-\vec{r}_8^{\,\prime})\,\delta(s_1,s_8')\,\delta(t_1,t_8') \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \delta(\vec{r}_8-\vec{r}_8^{\,\prime})\ \delta(s_8,s_1')\ \delta(t_8,t_1')\ ..\ \delta(\vec{r}_8-\vec{r}_8^{\,\prime})\ \delta(s_8,t_8')\ \delta(t_8,t_8') \end{vmatrix}$$

$$\times\ d\tau'\ \mathcal{O}\, G_{N\ell m}(\,...\vec{r}_i..\,)\ X(S,T)\ d\tau$$

where $\mathcal{O}$ is some operator that is symmetric in all particles (not a symmetrizing operator) and the integrals include a summation over the spin and isotopic spin coordinates.

Because operator $\mathcal{O}$ is symmetric in all particles,

$$\mathcal{O}\psi_{N\ell m} = \mathcal{O}\mathcal{A}\, G_{N\ell m}\, X = \mathcal{A}\, \mathcal{O}\, G_{N\ell m} X$$

Also from Appendix 7

$$(\mathcal{A}\, u)\ (\mathcal{A}\, v) = \mathcal{S}(u\mathcal{A}\, v)$$

where u and v are any functions of the eight position vectors. Hence,

$$\psi^*_{N\ell m}\ \mathcal{O}\psi_{N\ell m} = \mathcal{A}(G_{N\ell m}X)^*\ \mathcal{A}(\mathcal{O}\, G_{N\ell m}X) = \mathcal{S}(G^*_{N\ell m}X^*\mathcal{A}\mathcal{O}G_{N\ell m}X$$

$$= \mathcal{S}(G^*_{N\ell m}X^*\mathcal{O}\mathcal{A}\ G_{N\ell m}X) = \mathcal{S}\left[(\mathcal{A}G^*_{N\ell m}X^*)\ \ \mathcal{O}\, G_{N\ell m}X\right]$$

Therefore

$$\langle\mathcal{O}\rangle = \int \mathcal{S}\left[(\mathcal{A}\, G^*_{N\ell m}X^*)\ \ \mathcal{O}\, G_{N\ell m}X\right] d\tau$$

In addition it is shown in Appendix 7 that,

$$\int \mathcal{S} f(\vec{r}_1 \ldots \vec{r}_8)\ d\tau \ = \sqrt{\underset{8}{24}!}\ \int f(\vec{r}_1 \ldots \vec{r}_8)\ d\tau$$

$$\langle \mathcal{O} \rangle \ = \ \sqrt{\underset{8}{\cancel{24}}!} \int (\mathcal{A}\, G^*_{N\ell m} X^*)\ \mathcal{O}\, G_{N\ell m} X\ d\tau$$

$$= \iint G_{N\ell m}(\ldots \vec{r}'_i \ldots) X(S,T)'$$

$$\begin{vmatrix} \delta(\vec{r}_1 - \vec{r}'_1)\ \delta(s_1, s'_1)\ \delta(t_1, t'_1) \ldots & \delta(\vec{r}_1 - \vec{r}'_8)\ \delta(s_1, s'_8)\ \delta(t_1, t'_8) \\ \ldots\ldots\ldots\ldots\ldots\ldots & \ldots\ldots\ldots\ldots\ldots\ldots \\ \delta(\vec{r}_8 - \vec{r}'_1)\ \delta(s_8, s'_1)\ \delta(t_8, t'_1) \ldots & \delta(\vec{r}_8 - \vec{r}'_8)\ \delta(s_8, s'_8)\ \delta(t_8, t'_8) \end{vmatrix}$$

$$d\tau' \ \ \mathcal{O}\, G_{N\ell m}(\vec{r}_1 \ldots \vec{r}_8)\ X(S,T)\ d\tau$$

APPENDIX 12

The object of this appendix is to reduce the integrals I_1, I_2, I_3, I_4, I_5, and I_6 from page 31 to a simple form.

Consider the integral denoted by I_1: We have that

$$\psi(o) = \exp\left[-\frac{a}{2}\sum_{i=1}^{6}\beta_i^2\right]R^N \exp\left[-\beta R^2\right]Y_\ell^m(\Omega)$$

Therefore it follows that

$$I_1 = \int \exp\left[-a\sum_{i=1}^{6}\beta_i^2\right] R^{2N+1}\exp\left[-2\beta R^2\right]Y_\ell^m(\Omega)^* \, Y_\ell^m(\Omega)\, d\tau$$

Actually we are now only considering the seven independent vector variables excluding the center of mass variables. We are not interested in the center of mass motion and this is the reason that the center of mass dependence was dropped. However, as far as the calculation of expectation values are concerned the center of mass effect could just as well be left in the wave function and an integration over all eight independent vector coordinates performed. The reason is that the center of mass integral would be a common factor in both the numerator and denominator of equation (31). Hence, for simplicity, a center of mass function, $f(R_{cm})$, that satisfies the condition, $\int \left|f(R_{cm})\right|^2 d\tau_{cm}=1$, will be included. In terms of the cluster system of independent coordinates the integral, I_1, is written as follows:

$$I_1 = \int \exp\left[-a\sum_{i=1}^{6}\beta_i^2\right] R^{2N+1}\exp\left[-2\beta R^2\right]\left|Y_\ell^m(\Omega)\right|^2 J_1' \, d\vec{\beta}_1 \ldots d\vec{\beta}_6 \, d\vec{R}$$

where J_1' denotes the Jacobian associated with the transformation from the independent particle coordinate system to the cluster system of coordinates and is given by

$$J_1 = \begin{vmatrix} \frac{\partial x_1}{\partial \beta_{1_x}} & \frac{\partial x_1}{\partial \beta_{1_y}} & \frac{\partial x_1}{\partial \beta_{1_z}} & \frac{\partial x_1}{\partial \beta_{2_x}} & \cdots & \frac{\partial x_1}{\partial R_z} & \frac{\partial x_1}{\partial R_{cm_x}} & \frac{\partial x_1}{\partial R_{cm_y}} & \frac{\partial x_1}{\partial R_{cm_z}} \\ \frac{\partial y_1}{\partial \beta_{1_x}} & \cdots & & & & & & & \frac{\partial y_1}{\partial R_{cm_z}} \\ \cdots & & & & & & & & \cdots \\ \frac{\partial z_8}{\partial \beta_{1_x}} & \cdots & & & & & & & \frac{\partial z_8}{\partial R_{cm_z}} \end{vmatrix}$$

It is shown in Appendix 13 that:

$$J_1' = 2^6$$

Also it follows from

$$\int \exp\left[-a\beta^2\right] d\vec{\beta} = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \int_0^{\infty} \exp\left[-a\beta^2\right] \beta^2 \, d\beta = \left(\frac{\pi}{a}\right)^{\frac{3}{2}}$$

that

$$\int \exp\left[-a \sum_{i=1}^{6} \beta_i^2\right] d\vec{\beta}_1 \ldots d\vec{\beta}_6 = \frac{\pi^9}{a^9}$$

Since normalized spherical harmonics are being employed it finally follows that:

$$I_1 = \frac{\pi^9 2^6}{a^9} \int_0^{\infty} R^{2N+3} \exp\left[-2\beta R^2\right] dR \qquad \ldots(1)$$

Similarly

$$I_4 = \frac{\pi^9 2^6}{a^9} \int_0^{\infty} R^{2N+2} \exp\left[-2\beta R^2\right] dR \qquad \ldots(2)$$

Consider the integral denoted by I_2. We have that

$$\psi(48) = P_{48}\psi(o) = \int P_{48}\psi(o')\,\delta(\vec{r}_1-\vec{r}\,'_1)\,\delta(\vec{r}_2-\vec{r}\,'_2)\ldots\delta(\vec{r}_8-\vec{r}\,'_8)\;d\tau'$$

Therefore

$$I_2 = \int \exp\left[-\frac{a}{2}\sum_{i=1}^{8}\gamma_i^2\right] R^{N+1}\exp\left[-\beta R^2\right] Y_\ell^m(\Omega)\; f(R_{cm})\,d\tau$$

$$\int \exp\left[-\frac{a}{2}\sum_{i=1}^{8}\gamma_i'^2\right] R^N \exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')^* f(R_{cm})^* \qquad \ldots(3)$$

$$\delta(\vec{r}_1-\vec{r}\,'_1)\,\delta(\vec{r}_2-\vec{r}\,'_2)\,\delta(\vec{r}_3-\vec{r}\,'_3)\,\delta(\vec{r}_8-\vec{r}\,'_4)\,\delta(\vec{r}_5-\vec{r}\,'_5)\,\delta(\vec{r}_6-\vec{r}\,'_6)\,\delta(\vec{r}_7-\vec{r}\,'_7)\,\delta(\vec{r}_4-\vec{r}\,'_8)\,d\tau$$

Only six of the $\vec{\gamma}_i$ are independent variables. Choosing $\vec{\gamma}_2$, $\vec{\gamma}_3$, $\vec{\gamma}_4$ and $\vec{\gamma}_6$, $\vec{\gamma}_7$, $\vec{\gamma}_8$ for the independent internal variables, along with $\vec{R}$ and R_{cm}, the delta functions and elemental volumes are not transformed to this new set of independent variables.

The delta functions in equation (3) cause the following relationship between the primed and unprimed independent particle system of coordinates, $\vec{r}_1=\vec{r}\,'_1$, $\vec{r}_2=\vec{r}\,'_2$, $\vec{r}_3=\vec{r}\,'_3$, $\vec{r}_4=\vec{r}\,'_8$, $\vec{r}_5=\vec{r}\,'_5$, $\vec{r}_6=\vec{r}\,'_6$, $\vec{r}_7=\vec{r}\,'_7$, $\vec{r}_8=\vec{r}\,'_4$. From this relationship and the definition of $\vec{R}_{cm}$ on page 15 it follows that $\vec{R}_{cm}$ is equal to $\vec{R}\,'_{cm}$. Therefore one of the delta functions is $\delta(\vec{R}_{cm}-\vec{R}\,'_{cm})$. Also it follows immediately that $\vec{R} = \vec{R}\,' - \frac{\vec{r}\,'_4-\vec{r}\,'_8}{2} = \frac{\vec{R}\,'}{2} - \frac{\vec{\gamma}\,'_4-\vec{\gamma}\,'_8}{2}$ and hence another delta function is $\delta\left(\vec{R}-\frac{\vec{R}\,'}{2}+\frac{\vec{\gamma}\,'_4-\vec{\gamma}\,'_8}{2}\right)$

Next, the problem of integrating over the unprimed internal independent coordinates is considered. It is seen in equation (3) that the internal functional form involves the quantity

$$\sum_{i=1}^{8}\gamma_i^2$$

Using the relationship between the primed and unprimed independent particle coordinates, an algebraic manipulation gives the result

$$\sum_{i=1}^{8} \gamma_i^2 = \sum_{i=1}^{8} \gamma_i'^2 + 2(R'^2 - R^2)$$

Therefore equation (3) becomes

$$I_2 = J_2 \int \exp\left[-a\sum_{i=1}^{8} \gamma_i'^2 - a(R'^2 - R^2)\right] R^{N+1} \exp\left[-\beta R^2\right] Y_\ell^m(\Omega)\, R'^N$$

$$\exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')^*$$

$$\delta\left(\vec{R} - \frac{\vec{R}'}{2} + \frac{\vec{\gamma}_4' - \vec{\gamma}_8'}{2}\right) d\vec{\gamma}_2'\, d\vec{\gamma}_3'\, d\vec{\gamma}_4'\, d\vec{\gamma}_6'\, d\vec{\gamma}_7'\, d\vec{\gamma}_8'\, d\vec{R}\, d\vec{R}'$$

where J_2 is the Jacobian associated with the transformation from the $(\vec{r}_1', \vec{r}_2', \vec{r}_3', \vec{r}_4', \vec{r}_5', \vec{r}_6', \vec{r}_7', \vec{r}_8')$ system of coordinates to the $(\vec{\gamma}_2', \vec{\gamma}_3', \vec{\gamma}_4', \vec{\gamma}_6', \vec{\gamma}_7', \vec{\gamma}_8', \vec{R}', \vec{R}_{cm}')$ system of coordinates. In Appendix 14 it is shown that

$$J_2 = 2^{15}$$

The integration over the internal coordinates will now be performed. Consider the integral

$$I' = \int \exp\left[-a\sum_{i=1}^{8} \gamma_i'^2\right] \delta\left(\vec{R} - \frac{\vec{R}'}{2} + \frac{\vec{\gamma}_4' - \vec{\gamma}_8'}{2}\right) d\vec{\gamma}_2'\, d\vec{\gamma}_3'\, d\vec{\gamma}_4'\, d\vec{\gamma}_6'\, d\vec{\gamma}_7'\, d\vec{\gamma}_8'$$

This integral is evaluated in Appendix 15. The result is,

$$I' = \left[\frac{\pi^{15}}{3^3\, 2^9\, a^{15}}\right]^{\frac{1}{2}} \exp\left[-\frac{2a}{3}(\vec{R}' - 2\vec{R})^2\right]$$

Therefore

$$I_2=2^{12}\left[\frac{\pi^5}{6\ a^5}\right]^{\frac{3}{2}}\int \exp\left[-\ \frac{(5a+\beta)R^2}{3}+\frac{8a\vec{R}\cdot\vec{R}'}{3}-\frac{(5a+\beta)R'^2}{3}\right]$$

$$R^{N+3}\ R'^{N+2}\ \ Y_\ell^m\ (\Omega)\,Y_\ell^m(\Omega')^*\,dR\,dR'\,d\Omega\,d\Omega'$$

Similarly,

$$I_5=2^{12}\left[\frac{\pi^5}{6\ a^5}\right]^{\frac{3}{2}\cdot}\int \exp\left[-\frac{(5a+\beta)R^2}{3}+\frac{8a\vec{R}\cdot\vec{R}'}{3}-\frac{(5a+\beta)R'^2}{3}\right]$$

$$R^{N+2}\ R'^{N+2}\ \ Y_\ell^m(\Omega)\,Y_\ell^m(\Omega')^*\,dR\,dR'\,d\Omega\,d\Omega'$$

Consider next the integral denoted by I_3. We have that

$$\psi(37,48)=P_{48}P_{37}\psi(o)=\int P_{48}P_{37}\ \psi(o')\ \ \delta(\vec{r}_1-\vec{r}_1')\,\delta(\vec{r}_2-\vec{r}_2')\ldots\delta(\vec{r}_8-\vec{r}_8')\ \ d\tau'$$

Therefore,

$$I_3=\int \exp\left[-\ \frac{a}{2}\sum_{i=1}^{8}\gamma_i^2\right]R^{N+1}\ \ \exp\left[-\ \beta R^2\right]\ Y_\ell^m(\Omega)f(R_{cm})\ \ d\tau$$

$$\int \exp\left[-\ \frac{a}{2}\sum_{i=1}^{8}\gamma_i'^2\right]R'^N\ \ \exp\left[-\ \ \beta R'^2\right]Y_\ell^m(\Omega')^*$$

$$f(R'_{cm})^*\ \delta(\vec{r}_1-\vec{r}_1')\,\delta(\vec{r}_2-\vec{r}_2')\,\delta(\vec{r}_7-\vec{r}_3')\,\delta(\vec{r}_8-\vec{r}_4')\,\delta(\vec{r}_5-\vec{r}_5')\,\delta(\vec{r}_6-\vec{r}_6')$$

$$\delta(\vec{r}_3-\vec{r}_7')\,\delta(\vec{r}_4-\vec{r}_8')\ \ d\tau'$$

The set of independent variables that will be used here is $(\vec{\gamma}_2,\vec{\gamma}_3,\vec{\gamma}_4,\vec{\gamma}_6,\vec{\gamma}_7,\vec{\gamma}_8,\vec{R},\vec{R}_{cm})$. The delta functions in the above integral fix the following relationship between the primed and unprimed system of coordinates, $\vec{r}_1=\vec{r}\,'_1$, $\vec{r}_2=\vec{r}\,'_2$, $\vec{r}_7=\vec{r}\,'_3$, $\vec{r}_8=\vec{r}\,'_4$, $\vec{r}_5=\vec{r}\,'_5$, $\vec{r}_6=\vec{r}\,'_6$, $\vec{r}_3=\vec{r}\,'_7$, $\vec{r}_4=\vec{r}\,'_8$. It is seen immediately that $\vec{R}\,'_{cm}=\vec{R}_{cm}$. Hence one of the delta functions is $\delta(\vec{R}_{cm}-\vec{R}\,'_{cm})$. The use of the relationship between the primed and unprimed system of independent particle coordinates in a short algebraic manipulation gives,

$$\vec{R} = \frac{\vec{\Upsilon}\,'_7 + \vec{\Upsilon}\,'_8 - \vec{\Upsilon}\,'_3 - \vec{\Upsilon}\,'_4}{2}$$

Hence in this cluster system of coordinates another one of the delta functions is given by

$$\delta\left(\vec{R} - \frac{\vec{\Upsilon}\,'_7 + \vec{\Upsilon}\,'_8 - \vec{\Upsilon}\,'_3 - \vec{\Upsilon}\,'_4}{2}\right)$$

Next, the integration over the unprimed internal coordinates will be performed. Using the relationship between the primed and unprimed independent particle system of coordinates, an algebraic manipulation gives the result that,

$$\sum_{i=1}^{8} \vec{\Upsilon}_i^{2} = \sum_{i=1}^{8} \vec{\Upsilon}_i^{\prime 2} - 2\vec{R}^2 + 2\vec{R}^{\prime 2}$$

Therefore

$$I_3=2^{15}\int \exp\left[-a\sum_{i=1}^{8}\Upsilon_i^{\prime 2} - aR'^2 + aR^2\right] R^{N+1} \exp\left[-\beta R^2\right] Y_\ell^m(\Omega)$$
$$R'^N \exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')^* \; \delta\left(\vec{R}-\frac{\vec{\Upsilon}\,'_7+\vec{\Upsilon}\,'_8-\vec{\Upsilon}\,'_3-\vec{\Upsilon}\,'_4}{2}\right) d\vec{\Upsilon}\,'_2 d\vec{\Upsilon}\,'_3 d\vec{\Upsilon}\,'_4 d\vec{\Upsilon}\,'_6 d\vec{\Upsilon}\,'_7 d\vec{\Upsilon}\,'_8 d\vec{R} d\vec{R}$$

Next the integration over the primed internal coordinates will be performed

Consider the following integral

$$I'' = \int \exp\left[-a\sum_{i=1}^{8} \gamma_i'^2\right] \delta\left(\vec{R} - \frac{\vec{\gamma}_7' + \vec{\gamma}_8' - \vec{\gamma}_3' - \vec{\gamma}_4'}{2}\right) d\vec{\gamma}_2'\, d\vec{\gamma}_3'\, d\vec{\gamma}_4'\, d\vec{\gamma}_6'\, d\vec{\gamma}_7'\, d\vec{\gamma}_8'$$

This integral is evaluated in Appendix 16 and the result is

$$I'' = \left(\frac{\pi}{2a}\right)^{\frac{15}{2}} \exp\left[-2aR^2\right]$$

Therefore,

$$I_3 = 2^9 \left[\frac{\pi^5}{2a^5}\right]^{\frac{3}{2}} \int \exp\left[-aR'^2 - aR^2 - \beta R^2\right] R^{N+3}\, Y_\ell^m(\Omega)\, R'^{N+2}$$

$$\exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')^*\, dR\, dR'\, d\Omega\, d\Omega'$$

Similarly,

$$I_6 = 2^9 \left[\frac{\pi^5}{2a^5}\right]^{\frac{3}{2}} \int R^{N+2}\, R'^{N+2} \exp\left[-(a+\beta)R'^2 - (a+\beta)R^2\right] Y_\ell^m(\Omega)\, Y_\ell^m(\Omega')^*$$

$$dR\, dR'\, d\Omega\, d\Omega'$$

Next, the integral denoted by I_{10} is considered. From page we have that

$$I_{10} = \int \psi(48)\, \sigma(R)\, \psi(48)\, d\tau$$

This can also be written

$$I_{10} = \int \sigma(R)\, d\tau \int P_{48} \exp\left[-a \sum_{i=1}^{8} \gamma_i'^{\,2}\right] R'^{\,8} \exp\left[-2\beta R'^{\,2}\right] Y_\ell^m(\Omega')\, Y_\ell^m(\Omega')$$

$$\delta(\vec{r}_1 - \vec{r}_1{}')\dots\ \delta(\vec{r}_8 - \vec{r}_8{}')\, d\tau \quad .$$

Choosing $\vec{\gamma}_2, \vec{\gamma}_3, \vec{\gamma}_4, \vec{\gamma}_6, \vec{\gamma}_7, \vec{\gamma}_8$ for the independent internal variables, along with $\vec{R}$ and $\vec{R}_{cm}$, the delta functions are now transformed into this new set of independent variables. The delta functions in the preceeding equation cause the following relationship between the primed and unprimed independent particles system of coordinates; $\vec{r}_1 = \vec{r}\,'_1, \vec{r}_2 = \vec{r}\,'_2, \vec{r}_3 = \vec{r}\,'_3, \vec{r}_4 = \vec{r}\,'_8, \vec{r}_5 = \vec{r}\,'_5, \vec{r}_6 = \vec{r}\,'_6,$ $\vec{r}_7 = \vec{r}\,'_7, \vec{r}_8 = \vec{r}\,'_4$. Therefore it is seen that the center of mass coordinates are unchanged and one of the delta functions in the new system of coordinates is $\delta(\vec{R}_{cm} - \vec{R}_{cm}{}')$. Also it follows immediately that(see page)

$$\vec{R} = \frac{\vec{R}'}{2} - \frac{\vec{\gamma}\,'_4 - \vec{\gamma}\,'_8}{2}$$

Hence another delta function is $\delta\left(\vec{R} - \frac{\vec{R}'}{2} + \frac{\vec{\gamma}\,'_4 - \vec{\gamma}\,'_8}{2}\right)$. Now consider the problem of integrating over the unprimed internal coordinates. This involves changing all the primed internal coordinates by it's equivalent in the primed system of coordinates by the relationship between the primed and unprimed independent system of coordinates. Since $\sigma(R)$ is independent of the internal coordinates this transformation leaves $\sigma(R)$ unchanged and I_{10} becomes

$$I_{10} = 2^{15}\int \sigma(R)\exp\left[-a\sum_{i=1}^{8}\gamma_i'^{2}\right] R'^{2}\exp\left[-2\beta R'^{2}\right] Y_{\ell}^{m}(\Omega')\, Y_{\ell}^{m}(\Omega')$$

$$\delta\left(\vec{R}-\frac{\vec{R}'}{2}+\frac{\vec{\gamma}_4'-\vec{\gamma}_8'}{2}\right)d\vec{R}\,d\vec{\gamma}_2'\,d\vec{\gamma}_3'\,d\vec{\gamma}_4'\,d\vec{\gamma}_6'\,d\vec{\gamma}_7'\,d\vec{\gamma}_8'$$

But from Appendis 15,page , it follows that

$$I_{10} = 2^{15}\left[\frac{\pi^{15}}{3^{3}\cdot 2^{9}a^{15}}\right]^{\frac{1}{2}}\int \sigma(R)\exp\left[-\frac{2a}{3}(R'-2R)^{2}\right] R'^{8}\exp\left[-2\beta R'^{2}\right]$$

$$Y_{\ell}^{m}(\Omega')\, Y_{\ell}^{m}(\Omega')\,d\vec{R}\,d\vec{R}'$$

Rearranging this expression the integral becomes

$$I_{10} = \left[\frac{2^{21}\pi^{15}}{3^{3}a^{15}}\right]^{\frac{1}{2}} A\left(\frac{2a}{3}+2\ \ ,\frac{8a}{3},\frac{8a}{3}\right)$$

where

$$A(p,q,s)_{N\ell m} = \int \sigma(R)R'^{2N+2}R^{2}\exp\left[-pR'^{2}+q\vec{R}'\cdot\vec{R}-sR^{2}\right] Y_{\ell}^{m}(\Omega')\, Y_{\ell}^{m}(\Omega')\,dR\,dR'\,d\Omega\,d\Omega$$

The integrations involved in the preceeding expression are quite straight forward and the result is

$$A\left(\frac{2a}{3}+2\beta,\frac{8a}{3},\frac{8a}{3}\right) = \frac{7\cdot 5\cdot 3^{8+\frac{1}{2}}\pi^{2}}{2^{25}a^{8}\epsilon^{2+\frac{1}{2}}(1+3\epsilon)^{3}}\left[3+\frac{5}{3\epsilon}+\frac{7}{3\cdot 2^{3}\epsilon^{2}}+\frac{1}{2^{4}\cdot 3\epsilon^{3}}+\frac{11}{3^{4}\cdot 2^{8}\epsilon^{4}}\right]$$

when $\sigma(R) = R^{2}$ and the system is in the ground state.

Now, the integral denoted by I_{13} is considered. From page we have that

$$I_{13} = \int \psi(48,37)\sigma(R)\psi(48,37)\,d\tau$$

This and also be written

$$I_{13} = \int \sigma(R)\,d\tau \int P_{48}P_{37}\,\psi(o')^{*}\,\psi(o')\;\delta(\vec{r}_1 - \vec{r}\,'_1)\ldots\;\delta(\vec{r}_8 - \vec{r}\,'_8)\,d\tau'$$

Just as in the analysis of the last integration $\vec{\gamma}_2$, $\vec{\gamma}_3$, $\vec{\gamma}_4$, $\vec{\gamma}_6$, $\vec{\gamma}_7$, $\vec{\gamma}_8$, are chosen for the independent internal coordinates, along with $\vec{R}$ and $\vec{R}_{cm}$. The delta functions in the preceding equation cause the following relationship between the primed and unprimed independent particle system of coordinates; $\vec{r}_1 = \vec{r}\,'_1$, $\vec{r}_2 = \vec{r}\,'_2$, $\vec{r}_3 = \vec{r}\,'_7$, $\vec{r}_4 = \vec{r}\,'_8$, $\vec{r}_5 = \vec{r}\,'_5$, $\vec{r}_6 = \vec{r}\,'_6$, $\vec{r}_7 = \vec{r}\,'_3$, $\vec{r}_8 = \vec{r}\,'_4$. Once again the center of mass coordinates is the same in primed and the unprimed system of variables. Also it follows from page that another delta function in the cluster system of coordinates is $\delta\left(\vec{R} - \frac{\vec{\gamma}\,'_7 + \vec{\gamma}\,'_8 - \vec{\gamma}\,'_3 - \vec{\gamma}\,'_4}{2}\right)$. Next the integration over the unprimed internal coordinates is performed. The equivalent of this integration is the transformation of the unprimed internal coordinates (due to the delta functions) in the primed system of coordinates. Since $\sigma(R)$ is not dependent upon the internal coordinates this integration leaves $\sigma(R)$ unchanged and I_{13} becomes

$$I_{13} = 2^{15}\int \sigma(R)\exp\left[-a\sum_{i=1}^{8}\gamma'^{2}_{i}\right] R'^{8}\exp\left[-2\beta R'^{2}\right] Y_{\ell}^{m}(\Omega')^{*}\, Y_{\ell}^{m}(\Omega')\,d\vec{R}\,'\,d\vec{R}$$
$$\delta\left(\vec{R} - \frac{\vec{\gamma}\,'_7 + \vec{\gamma}\,'_8 - \vec{\gamma}\,'_3 - \vec{\gamma}\,'_4}{2}\right) d\vec{\gamma}\,'_2\, d\vec{\gamma}\,'_3\, d\vec{\gamma}\,'_4\, d\vec{\gamma}\,'_6\, d\vec{\gamma}\,'_7\, d\vec{\gamma}\,'_8$$

It now follows from the results of Appendix 16 that

$$I_{13} = \left[\frac{2\pi}{a}\right]^{\frac{15}{2}} \int \sigma(R) R'^{8} \exp\left[-2\beta R'^{2} - 2aR^{2}\right] Y_{\ell}^{m}(\Omega')^{*} Y_{\ell}^{m}(\Omega') \, d\vec{R}' \, d\vec{R}$$

and since the spherical harmonics are normalized it follows that for $\sigma(R) = R^2$

$$I_{13} = \frac{7 \cdot 5 \cdot 3^{3} \pi^{9}}{2^{2} \epsilon^{5+\frac{1}{2}} a^{13}} \int_{0}^{\infty} R^{4} \exp\left[-2aR^{2}\right] dR$$

Consider the following integral

$$I_{14} = \int \psi(48,26)^{*} \sigma(R) \psi(48,37) d\tau$$

This integral can be simplified by writing it as follows

$$I_{14} = \int \sigma(R) d\tau \left[\int P_{48} P_{26} \psi(o')^{*} \delta(\vec{r}_1 - \vec{r}\,'_1) \ldots \delta(\vec{r}_8 - \vec{r}\,'_8) d\tau' \right]$$

$$\int P_{48} P_{37} \psi(o'') \delta(\vec{r}_1 - \vec{r}\,''_1) \ldots \delta(\vec{r}_8 - \vec{r}\,''_8) d\tau''$$

The delta functions in this equation cause the following relationship between the double primed, the primed, and the unprimed independent particles system of coordinates; $\vec{r}_1 = \vec{r}\,'_1 = \vec{r}\,''_1$, $\vec{r}_2 = \vec{r}\,'_6 = \vec{r}\,''_2$, $\vec{r}_3 = \vec{r}\,'_3 = \vec{r}\,''_7$, $\vec{r}_4 = \vec{r}\,'_8 = \vec{r}\,''_8$, $\vec{r}_5 = \vec{r}\,'_5 = \vec{r}\,''_5$, $\vec{r}_6 = \vec{r}\,'_2 = \vec{r}\,''_6$, $\vec{r}_7 = \vec{r}\,'_7 = \vec{r}\,''_3$, $\vec{r}_8 = \vec{r}\,'_4 = \vec{r}\,''_4$. From this relationship it is seen that $\vec{R}_{cm} = \vec{R}'_{cm} = \vec{R}''_{cm}$. Hence two of the delta functions are $\delta(\vec{R}_{cm} - \vec{R}'_{cm})$ and $\delta(\vec{R}_{cm} - \vec{R}''_{cm})$. Also it is seen from page that another two delta functions in the cluster system of coordinates are

$$\delta\left(\vec{R} - \frac{\vec{\gamma}\,'_6 + \vec{\gamma}\,'_8 - \vec{\gamma}\,'_2 - \vec{\gamma}\,'_4}{2}\right) \text{ and } \delta\left(\vec{R} - \frac{\vec{\gamma}\,''_7 + \vec{\gamma}\,''_8 - \vec{\gamma}\,''_3 - \vec{\gamma}\,''_7}{2}\right).$$

Furthermore the above relationships require that

$$\vec{\gamma}_1 = \vec{\gamma}\,'_1 - \frac{\vec{R}}{2} + \frac{\vec{R}'}{2}; \quad \vec{\gamma}_1 = \vec{\gamma}\,''_1 - \frac{\vec{R}}{2} + \frac{\vec{R}''}{2}; \quad \vec{\gamma}_5 = \vec{\gamma}\,'_5 + \frac{\vec{R}}{2} - \frac{\vec{R}'}{2}; \quad \vec{\gamma}_5 = \vec{\gamma}\,''_5 + \frac{\vec{R}}{2} - \frac{\vec{R}''}{2}$$

$$\vec{\gamma}_2 = \vec{\gamma}\,'_6 - \frac{\vec{R}}{2} - \frac{\vec{R}'}{2}; \quad \vec{\gamma}_2 = \vec{\gamma}\,''_2 - \frac{\vec{R}}{2} + \frac{\vec{R}''}{2}; \quad \vec{\gamma}_6 = \vec{\gamma}\,'_2 + \frac{\vec{R}}{2} + \frac{\vec{R}'}{2}; \quad \vec{\gamma}_6 = \vec{\gamma}\,''_6 + \frac{\vec{R}}{2} - \frac{\vec{R}''}{2}$$

$$\vec{\gamma}_3 = \vec{\gamma}\,'_3 - \frac{\vec{R}}{2} + \frac{\vec{R}'}{2}; \quad \vec{\gamma}_3 = \vec{\gamma}\,''_7 - \frac{\vec{R}}{2} - \frac{\vec{R}''}{2}; \quad \vec{\gamma}_7 = \vec{\gamma}\,'_7 + \frac{\vec{R}}{2} - \frac{\vec{R}'}{2}; \quad \vec{\gamma}_7 = \vec{\gamma}\,''_3 + \frac{\vec{R}}{2} + \frac{\vec{R}''}{2}$$

$$\vec{\gamma}_4 = \vec{\gamma}\,'_8 - \frac{\vec{R}}{2} - \frac{\vec{R}'}{2}; \quad \vec{\gamma}_4 = \vec{\gamma}\,''_8 - \frac{\vec{R}}{2} - \frac{\vec{R}''}{2}; \quad \vec{\gamma}_8 = \vec{\gamma}\,'_4 + \frac{\vec{R}}{2} + \frac{\vec{R}'}{2}; \quad \vec{\gamma}_8 = \vec{\gamma}\,''_4 + \frac{\vec{R}}{2} + \frac{\vec{R}''}{2}$$

From these relations it is seen that an integration over the unprimed internal coordinates yields the following*

$$I_{14} = 2^{15}\int \sigma(R)\,d\vec{R}\int \psi(o')\,\delta\Big(\vec{R} - \frac{\vec{\gamma}'_6 + \vec{\gamma}'_8 - \vec{\gamma}'_2 - \vec{\gamma}'_4}{2}\Big)\,d\vec{R}'\,d\vec{\gamma}'_2\,d\vec{\gamma}'_3\,d\vec{\gamma}'_4\,d\vec{\gamma}'_6$$

$$d\gamma'_7\,d\gamma'_8\int \psi(o'')\,\delta(2\vec{R} - \vec{\gamma}''_7 - \vec{\gamma}''_8 + \vec{\gamma}''_3 + \vec{\gamma}''_4)\,\delta\Big(\vec{\gamma}''_2 - \vec{\gamma}'_6 + \frac{\vec{R}'}{2} + \frac{\vec{R}''}{2}\Big)$$

$$\delta\Big(\vec{\gamma}''_3 - \vec{\gamma}'_7 + \frac{\vec{R}'}{2} + \frac{\vec{R}''}{2}\Big)\,\delta\Big(\vec{\gamma}''_4 - \vec{\gamma}'_4 - \frac{\vec{R}'}{2} + \frac{\vec{R}''}{2}\Big)\,\delta\Big(\vec{\gamma}''_6 - \vec{\gamma}'_2 - \frac{\vec{R}'}{2} - \frac{\vec{R}''}{2}\Big)$$

$$\delta\Big(\vec{\gamma}''_7 - \vec{\gamma}'_3 - \frac{\vec{R}'}{2} - \frac{\vec{R}''}{2}\Big)\,\delta\Big(\vec{\gamma}''_8 - \vec{\gamma}'_8 + \frac{\vec{R}'}{2} - \frac{\vec{R}''}{2}\Big)\,d\vec{\gamma}''_2\,d\vec{\gamma}''_3\,d\vec{\gamma}''_4\,d\vec{\gamma}''_6\,d\vec{\gamma}''_7\,d\vec{\gamma}''_8\,d\vec{R}''$$

Next the integration over the double primed internal coordinates is performed. Since only six of the eight variables are independent and because ($\vec{\gamma}_2, \vec{\gamma}_3, \vec{\gamma}_4, \vec{\gamma}_6, \vec{\gamma}_7, \vec{\gamma}_8, \vec{R}, \vec{R}_{cm}$) have been taken for the set of independent vector variables it is now necessary to eliminate the vectors $\vec{\gamma}_1$, and $\vec{\gamma}_5$ by writing them in terms of the independent variables. From Appendix 2 it follows that $\gamma_1^2 = (\vec{\gamma}_2 + \vec{\gamma}_3 + \vec{\gamma}_4)^2$ and $\gamma_5^2 = (\vec{\gamma}_6 + \vec{\gamma}_7 + \vec{\gamma}_8)^2$. The integration over the double primed internal coordinates can now be performed. This amounts to performing the following series of substitutions;

$$\delta\Big(\vec{\gamma}''_2 - \vec{\gamma}'_6 + \frac{\vec{R}'}{2} + \frac{\vec{R}''}{2}\Big)\,d\vec{\gamma}''_2 = 1 \qquad \vec{\gamma}''_2 = \vec{\gamma}'_6 - \frac{\vec{R}'}{2} - \frac{\vec{R}''}{2}$$

$$\delta\Big(\vec{\gamma}''_6 - \vec{\gamma}'_2 - \frac{\vec{R}'}{2} - \frac{\vec{R}''}{2}\Big)\,d\vec{\gamma}''_6 = 1 \qquad \vec{\gamma}''_6 = \vec{\gamma}'_2 + \frac{\vec{R}'}{2} + \frac{\vec{R}''}{2}$$

* It is easily shown that when ($\vec{\gamma}_2, \vec{\gamma}_3, \vec{\gamma}_4, \vec{\gamma}_6, \vec{\gamma}_7, \vec{\gamma}_8, \vec{R}, \vec{R}_{cm}$) are taken for the independent variables, it is redundant to include the following delta functions $\delta\Big(\vec{\gamma}_1 - \vec{\gamma}'_1 + \frac{\vec{R}}{2} - \frac{\vec{R}'}{2}\Big)$, $\delta\Big(\vec{\gamma}_1 - \vec{\gamma}''_1 + \frac{\vec{R}}{2} - \frac{\vec{R}''}{2}\Big)$ $\delta\Big(\vec{\gamma}_5 - \vec{\gamma}'_5 - \frac{\vec{R}}{2} + \frac{\vec{R}'}{2}\Big)$, $\delta\Big(\vec{\gamma}_5 - \vec{\gamma}''_5 - \frac{\vec{R}}{2} + \frac{\vec{R}''}{2}\Big)$

$$\delta(\vec\gamma''_3 - \vec\gamma'_7 + \frac{\vec R'}{2} + \frac{\vec R''}{2})\, d\vec\gamma''_3 = 1 \qquad \vec\gamma''_3 = \vec\gamma'_7 - \frac{\vec R'}{2} - \frac{\vec R''}{2}$$

$$\delta(\vec\gamma''_7 - \vec\gamma'_3 - \frac{\vec R'}{2} - \frac{\vec R''}{2})\, d\vec\gamma''_7 = 1 \qquad \vec\gamma''_7 = \vec\gamma'_3 + \frac{\vec R'}{2} + \frac{\vec R''}{2}$$

$$\delta(\vec\gamma''_4 - \vec\gamma'_4 - \frac{\vec R'}{2} + \frac{\vec R''}{2})\, d\vec\gamma''_4 = 1 \qquad \vec\gamma''_4 = \vec\gamma'_4 + \frac{\vec R'}{2} - \frac{\vec R''}{2}$$

$$\delta(\vec\gamma''_8 - \vec\gamma'_8 + \frac{\vec R'}{2} - \frac{\vec R''}{2})\, d\vec\gamma''_8 = 1 \qquad \vec\gamma''_8 = \vec\gamma'_8 - \frac{\vec R'}{2} + \frac{\vec R''}{2}$$

As a result of the preceding substitutions and performing the integration over $\vec\gamma'_4$ and $\vec\gamma'_2$, I_{14} becomes

$$\begin{aligned}
I_{14} = {} & 2^{15}\int \mathcal{O}(R)\, d\vec R \int R'^4 \exp\left[-\beta R'^2\right] Y_\ell^m(\Omega') \int R''^4 \exp\left[-\beta R''^2\right] Y_\ell^m(\Omega'') \\
& \exp\Big[-\tfrac{1}{2}a\Big\{(\vec\gamma'_6 - 2\vec R + \vec\gamma'_3 + \vec\gamma'_8)^2 + (\vec\gamma'_6 + \vec\gamma'_7 - \vec\gamma'_3 - 2\vec R'')^2 + \gamma'^2_3 \\
& + (2\vec R'' - 2\vec R + \vec\gamma'_3 - \vec\gamma'_7 + \vec\gamma'_8)^2 + (\vec\gamma'_6 + \vec\gamma'_7 + \vec\gamma'_8)^2 + \gamma'^2_6 + \gamma'^2_7 + \gamma'^2_8 \\
& + (\vec\gamma'_6 + \vec\gamma'_3 + \vec\gamma'_8 - 2\vec R + \frac{\vec R''}{2} - \frac{\vec R'}{2})^2 + (\vec\gamma'_6 - \frac{\vec R'}{2} - \frac{\vec R''}{2})^2 + (\vec\gamma'_7 - \frac{\vec R'}{2} - \frac{\vec R''}{2})^2 \\
& + (\frac{3\vec R''}{2} - 2\vec R + \frac{\vec R'}{2} + \vec\gamma'_3 - \vec\gamma'_7 + \vec\gamma'_8)^2 + (\vec\gamma'_3 + \frac{\vec R'}{2} + \frac{\vec R''}{2})^2 + (\vec\gamma'_8 - \frac{\vec R'}{2} + \frac{\vec R''}{2})^2 \\
& + (\vec\gamma'_6 + \vec\gamma'_7 + \vec\gamma'_8 - \frac{\vec R''}{2} + \frac{\vec R'}{2})^2 + (\vec\gamma'_6 + \vec\gamma'_7 - \vec\gamma'_3 - \frac{3\vec R''}{2} + \frac{\vec R'}{2})^2\Big\}\Big]\, d\vec R'\, d\vec R''\, d\vec\gamma'_3\, d\vec\gamma'_6 \\
& d\vec\gamma'_7\, d\vec\gamma'_8
\end{aligned}$$

Next the integration over $\vec\gamma'_6$ will be performed. In the last expression for I_{14} one can see that there are eight terms, internal to the second set of brackets of the last exponential, that are squared and contain the term $\vec\gamma'_6$. It can easily be shown that these terms can be replaced by the following more convenient equivalent set of terms

$$8\left[\vec{\gamma}'_6 + \frac{\vec{\gamma}'_7 + \vec{\gamma}'_8 - \vec{R} - \vec{R}''}{2}\right]^2 - 2(\vec{\gamma}'_7 + \vec{\gamma}'_8 - \vec{R} - \vec{R}'')^2 + (\vec{\gamma}'_3 + \vec{\gamma}'_8 - 2\vec{R})^2$$
$$+ (\vec{\gamma}'_7 - \vec{\gamma}'_3 - 2\vec{R}'')^2 + (\vec{\gamma}'_7 + \vec{\gamma}'_8)^2 + (\vec{\gamma}'_3 + \vec{\gamma}'_8 - 2\vec{R} + \frac{\vec{R}''}{2} - \frac{\vec{R}'}{2})^2$$
$$+ (\frac{\vec{R}'}{2} + \frac{\vec{R}''}{2})^2 + (\vec{\gamma}'_7 + \vec{\gamma}'_8 - \frac{\vec{R}''}{2} + \frac{\vec{R}'}{2})^2 + (\vec{\gamma}'_7 - \vec{\gamma}'_3 - \frac{3\vec{R}''}{2} + \frac{\vec{R}'}{2})^2$$

Also it is clear that

$$\int \exp\left[-4a\left\{\vec{\gamma}'_6 + \frac{\vec{\gamma}'_7 + \vec{\gamma}'_8 - \vec{R} - \vec{R}''}{2}\right\}^2\right] d\vec{\gamma}'_6 = \left[\frac{\pi}{4a}\right]^{\frac{3}{2}}$$

Performing the integration over $\vec{\gamma}'_6$, collecting and rearranging the $\vec{\gamma}'_8$ terms and then performing the integration over $\vec{\gamma}'_8$ yields the result

$$I_{14} = \frac{2^{12}\pi^3}{3^{1+\frac{1}{2}}a^3} \int \sigma(R)\,d\vec{R} \int R'^4 \exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')\,d\vec{R}' \int R''^4 \exp\left[-\beta R''^2\right] Y_\ell^m(\Omega'')\,d\vec{R}''$$
$$\exp\left[-\tfrac{1}{2}a\left\{\gamma_3'^2 + \gamma_7'^2 + (\vec{\gamma}'_7 - \frac{\vec{R}'}{2} - \frac{\vec{R}''}{2})^2 + (\vec{\gamma}'_3 + \frac{\vec{R}'}{2} + \frac{\vec{R}''}{2})^2 + (\vec{\gamma}'_7 - \vec{\gamma}'_3 - 2\vec{R}'')^2\right.\right.$$
$$+ (\frac{\vec{R}'}{2} + \frac{\vec{R}''}{2})^2 + (\vec{\gamma}'_7 - \vec{\gamma}'_3 - \frac{3\vec{R}''}{2} + \frac{\vec{R}'}{2})^2 - \frac{2}{3}(3\vec{R}'' - 3\vec{R} + 2\vec{\gamma}'_3 - \vec{\gamma}'_7)^2$$
$$+ (2\vec{R}'' - 2\vec{R} + \vec{\gamma}'_3 - \vec{\gamma}'_7)^2 + (\frac{3\vec{R}''}{2} - 2\vec{R} + \frac{\vec{R}'}{2} + \vec{\gamma}'_3 - \vec{\gamma}'_7)^2 + (\frac{\vec{R}''}{2} - \frac{\vec{R}'}{2})^2 + \gamma_7'^2$$
$$- 2(\vec{\gamma}'_7 - \vec{R} - \vec{R}'')^2 + (\vec{\gamma}'_3 - 2\vec{R})^2 + (\vec{\gamma}'_3 - 2\vec{R} + \frac{\vec{R}''}{2} - \frac{\vec{R}'}{2})^2 +$$
$$\left.\left.(\vec{\gamma}'_7 - \frac{\vec{R}''}{2} + \frac{\vec{R}'}{2})^2\right\}\right] d\vec{\gamma}'_3\, d\vec{\gamma}'_7$$

From the symmetry of the system one would expect a certain pattern associated with interchanging $\vec{\gamma}'_3$ and $\vec{\gamma}'_7$. It is easily seen that the expression for I_{14} is invariant with respect to an interchange of $\vec{\gamma}'_3$ and $\vec{\gamma}'_7$ if at the same time their signs are reversed. At certain stages of the calculations a watchful eye for patterns associated with the intermediate results, along with checks by thorough independ calculations makes it possible for one to obtain reliable results.

Grouping the $\vec{\gamma}_3'$ terms into a convenient form, performing the integration over $\vec{\gamma}_3'$, then after grouping and integrating over $\vec{\gamma}_7'$, I_{14} becomes

$$I_{14} = \frac{2^4 \pi^5}{a^6} \int \sigma(R) \exp\left[-2aR^2\right] d\vec{R} \int R'^4 \exp\left[-(\beta + a)R'^2\right] d\vec{R}' \, R''^4 \exp\left[-(\beta + a)R''^2\right] d\vec{R}''$$

or

$$I_{14} \quad \frac{2^2 \cdot 3^2 \cdot 5^2 \pi^9}{a^{13} (1+\epsilon)^7} \int_0^\infty \sigma(R) \, R^2 \exp\left[-2aR^2\right] dR$$

The integrations involved in the term denoted by I_{12} have been performed

$$I_{12} = \int \psi(48,37) \sigma(R) \psi(26) \, d\tau$$

The procedure for solving this term is similar to that method which led to the solution of I_{14}. The procedure is perhaps more tedious but the general method of solution is the same. For this reason the result for $\sigma(R)$ will be stated.

$$I_{12} = \frac{2^{7+\frac{1}{2}} \pi^6}{a^6} \int \sigma(R) \, d\vec{R} \int R'^4 \exp\left[-\beta R'^2\right] Y_\ell^m(\Omega') \, d\vec{R} \int R''^4 \exp\left[-\beta R''^2\right] Y_\ell^m(\Omega'') \, dR''$$
$$\exp\left[-a\left\{3R^2 - 4\vec{R}\cdot\vec{R}'' - 2\vec{R}\cdot\vec{R}' + 4\vec{R}''\cdot\vec{R}' + 2R'^2 + 3R''^2\right\}\right.$$

and finally for $\sigma(R) = R^2$

$$I_{12} = \frac{2^{6+\frac{1}{2}}\pi^{7+\frac{1}{2}}}{3^{3+\frac{1}{2}} \cdot a^{8+\frac{1}{2}}} \left[3^2 J(p,q,p) + 10a\mathcal{L}(p,q,p) - 8aT(p,q,p) \right]$$

where

$$p = \frac{5a}{3} + \beta \qquad q = \frac{8a}{3}$$

Also the integrations involved in the term denoted by I_{11} have been performed.

$$I_{11} = \int \psi(48)\sigma(R)\psi(37)\,d\tau$$

The result will now be stated.

$$I_{11} = \frac{2^{7+\frac{1}{2}}\pi^6}{a^6} \int R'^4 \exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')\,d\vec{R}' \int R''^4 \exp\left[-\beta R''^2\right] Y_\ell^m(\Omega'')\,d\vec{R}''$$
$$\int \sigma(R) \exp\left[-a\left\{4R^2 - 4\vec{R}\cdot\vec{R}'' - 4\vec{R}\cdot\vec{R}' + 2\vec{R}''\cdot\vec{R}' + 2R''^2 + 2R'^2\right\}\right]$$

and finally for $\sigma(R) = R^2$

$$I_{11} = \frac{3 \cdot 2^{1+\frac{1}{2}}\pi^{7+\frac{1}{2}}}{a^{8+\frac{1}{2}}} \left[J(\beta + a, 0, \beta + a) + \frac{4a}{3}\mathcal{L}(\beta + a, 0, \beta + a) \right]$$

APPENDIX 13

The purpose of this appendix is to evaluate the Jacobian associated with the following change of variables,

$$(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_6,\vec{r}_7,\vec{r}_8) \quad (\vec{\beta}_1,\vec{\beta}_2,\vec{\beta}_3,\vec{\beta}_4,\vec{\beta}_5,\vec{\beta}_6,\vec{R},\vec{R}_{cm})$$

The Jacobian is written down explicitly on page 90

First the $\vec{\beta}_i$ will be written in terms of the $\vec{r}_i$. From the definition of the coordinates, already given, it follows that:

$$\vec{\beta}_1=\frac{\vec{r}_2+\vec{r}_3-\vec{r}_1-\vec{r}_4}{2},\quad \vec{\beta}_2=\frac{\vec{r}_3+\vec{r}_1-\vec{r}_2-\vec{r}_4}{2},\quad \vec{\beta}_3=\frac{\vec{r}_1+\vec{r}_2-\vec{r}_4-\vec{r}_4}{2}$$

$$\vec{\beta}_4=\frac{\vec{r}_6+\vec{r}_7-\vec{r}_5-\vec{r}_8}{2},\quad \vec{\beta}_5=\frac{\vec{r}_7+\vec{r}_5-\vec{r}_6-\vec{r}_8}{2},\quad \vec{\beta}_6=\frac{\vec{r}_5+\vec{r}_6-\vec{r}_7-\vec{r}_8}{2},$$

$$\vec{R}=\frac{\vec{r}_1+\vec{r}_2+\vec{r}_3+\vec{r}_4-\vec{r}_5-\vec{r}_6-\vec{r}_7-\vec{r}_8}{4},\quad \vec{R}_{cm}=\frac{\vec{r}_1+\vec{r}_2+\vec{r}_3+\vec{r}_4+\vec{r}_5+\vec{r}_6+\vec{r}_7+\vec{r}_8}{8}$$

Now solving for the $\vec{r}_i$ in terms of the given cluster system of variables (this is made particularly simple by employing the associated augmented matrix (Reference 10)) gives the result:

$$\vec{r}_1=\frac{2\vec{R}_{cm}+\vec{R}-\vec{\beta}1+\vec{\beta}2+\vec{\beta}3}{2},\qquad \vec{r}_2=\frac{2\vec{R}_{cm}+\vec{R}+\vec{\beta}1-\vec{\beta}2+\vec{\beta}3}{2}$$

$$\vec{r}_3=\frac{2\vec{R}_{cm}+\vec{R}+\vec{\beta}1+\vec{\beta}2-\vec{\beta}3}{2},\qquad \vec{r}_4=\frac{2\vec{R}_{cm}+\vec{R}-\vec{\beta}1-\vec{\beta}2-\vec{\beta}3}{2}$$

$$\vec{r}_5=\frac{2\vec{R}_{cm}-\vec{R}-\vec{\beta}4+\vec{\beta}5+\vec{\beta}6}{2},\qquad \vec{r}_6=\frac{2\vec{R}_{cm}-\vec{R}+\vec{\beta}4-\vec{\beta}5+\vec{\beta}6}{2}$$

$$\vec{r}_7=\frac{2\vec{R}_{cm}-\vec{R}+\vec{\beta}4+\vec{\beta}5-\vec{\beta}6}{2},\qquad \vec{r}_8=\frac{2\vec{R}_{cm}-\vec{R}-\vec{\beta}4-\vec{\beta}5-\vec{\beta}6}{2}$$

It then follows that

$$J_1 = 2^6$$

APPENDIX 14

The object of this appendix is to evaluate the Jacobian associated with the following change of variables,

$$(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5,\vec{r}_6,\vec{r}_7,\vec{r}_8) \rightarrow (\vec{\gamma}_2,\vec{\gamma}_3,\vec{\gamma}_4,\vec{\gamma}_6,\vec{\gamma}_7,\vec{\gamma}_8,\vec{R},\vec{R}_{cm})$$

The Jacobian is given by the following expression:

$$J_2 = \begin{vmatrix} \frac{\partial x_1}{\partial \gamma_{2_x}} & \frac{\partial x_1}{\partial \gamma_{2_y}} & \frac{\partial x_1}{\partial \gamma_{2_z}} & \frac{\partial x_1}{\partial \gamma_{3_x}} & \cdots & \frac{\partial x_1}{\partial R_z} & \frac{\partial x_1}{\partial R_{cm_x}} & \frac{\partial x_1}{\partial R_{cm_y}} & \frac{\partial x_1}{\partial R_{cm_z}} \\ \frac{\partial y_1}{\partial \gamma_{2_x}} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \frac{\partial y_1}{\partial R_{cm_z}} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{\partial z_8}{\partial \gamma_{2_x}} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \frac{\partial z_8}{\partial R_{cm_z}} \end{vmatrix}$$

First the $\vec{\gamma}_i$ will be written in terms of the $\vec{r}_i$. From the definition of the coordinates already given, it follows immediately that:

$$\vec{\gamma}_2 = \frac{3\vec{r}_2-\vec{r}_1-\vec{r}_3-\vec{r}_4}{4}, \quad \vec{\gamma}_3 = \frac{3\vec{r}_3-\vec{r}_1-\vec{r}_2-\vec{r}_4}{4}, \quad \vec{\gamma}_4 = \frac{3\vec{r}_4-\vec{r}_1-\vec{r}_2-\vec{r}_3}{4}$$

$$\vec{\gamma}_6 = \frac{3\vec{r}_6-\vec{r}_5-\vec{r}_7-\vec{r}_8}{4} \quad \vec{\gamma}_7 = \frac{3\vec{r}_7-\vec{r}_5-\vec{r}_6-\vec{r}_8}{4} \quad \vec{\gamma}_8 = \frac{3\vec{r}_8-\vec{r}_5-\vec{r}_6-\vec{r}_7}{4}$$

Also

$$\vec{R} = \frac{\vec{r}_1+\vec{r}_2+\vec{r}_3+\vec{r}_4-\vec{r}_5-\vec{r}_6-\vec{r}_7-\vec{r}_8}{4}, \quad \vec{R}_{cm} = \frac{\vec{r}_1+\vec{r}_2+\vec{r}_3+\vec{r}_4+\vec{r}_5+\vec{r}_6+\vec{r}_7+\vec{r}_8}{8}$$

Now solving for the $\vec{r}_i$ in terms of the given cluster system of variables gives the result:

$$\vec{r}_1 = \frac{2\vec{R}_{cm}+\vec{R}-2(\vec{\gamma}_2+\vec{\gamma}_3+\vec{\gamma}_4)}{2} \quad \vec{r}_2 = \frac{2\vec{R}_{cm}+\vec{R}+2\vec{\gamma}_2}{2} \quad \vec{r}_3 = \frac{2\vec{R}_{cm}+\vec{R}+2\vec{\gamma}_3}{2}$$

$$\vec{r}_4 = \frac{2\vec{R}_{cm}+\vec{R}+2\vec{\gamma}_4}{2}, \quad \vec{r}_5 = \frac{2\vec{R}_{cm}-\vec{R}-2(\vec{\gamma}_6+\vec{\gamma}_7+\vec{\gamma}_8)}{2}, \quad \vec{r}_6 = \frac{2\vec{R}_{cm}-\vec{R}+2\vec{\gamma}_6}{2}$$

$$\vec{r}_7 = \frac{2\vec{R}_{cm}-\vec{R}+2\vec{\gamma}_7}{2}, \quad \vec{r}_8 = \frac{2\vec{R}_{cm}-\vec{R}+2\vec{\gamma}_8}{2}$$

Therefore

$$J_2 = 2^{15}$$

APPENDIX 15

The object of this appendix is to evaluate the following integral:

$$I' = \exp\left[-a\sum_{i=1}^{8}\Upsilon_i'^2\right]\delta\left(\vec{R}-\frac{\vec{R}'}{2}+\frac{\vec{\Upsilon}'_4-\vec{\Upsilon}'_8}{2}\right) d\vec{\Upsilon}'_2 d\vec{\Upsilon}'_3 d\vec{\Upsilon}'_6 d\vec{\Upsilon}'_7 d\vec{\Upsilon}'_8$$

From Appendix 2 we have that,

$$\Upsilon_1^2 = (\vec{\Upsilon}_2+\vec{\Upsilon}_3+\vec{\Upsilon}_4)^2 \text{ and } \Upsilon_5^2 = (\vec{\Upsilon}_6+\vec{\Upsilon}_7+\vec{\Upsilon}_8)^2 .$$

Therefore

$$I' = \exp\left[-a\left\{\Upsilon_2'^2+\Upsilon_3'^2+\Upsilon_4'^2+(\vec{\Upsilon}_2+\vec{\Upsilon}_3+\vec{\Upsilon}_4)^2\right\}\right]\exp\left[-a\left\{\Upsilon_6'^2+\Upsilon_7'^2+\Upsilon_8'^2+(\vec{\Upsilon}_6+\vec{\Upsilon}_7+\vec{\Upsilon}_8)^2\right\}\right]$$

$$\delta\left(\vec{R}-\frac{\vec{R}'}{2}+\frac{\vec{\Upsilon}'_4-\vec{\Upsilon}'_8}{2}\right) d\vec{\Upsilon}'_2 d\vec{\Upsilon}'_3 d\vec{\Upsilon}'_4 d\vec{\Upsilon}'_6 d\vec{\Upsilon}'_7 d\vec{\Upsilon}'_8$$

But,

$$\Upsilon_2^2+\Upsilon_3^2+\Upsilon_4^2 = 2\left[\vec{\Upsilon}_2+\frac{\vec{\Upsilon}_3+\vec{\Upsilon}_4}{2}\right]^2+\frac{(\vec{\Upsilon}_3+\vec{\Upsilon}_4)^2}{2}+\Upsilon_3^2+\Upsilon_4^2$$

$$\Upsilon_6^2+\Upsilon_7^2+\Upsilon_8^2 = 2\left[\vec{\Upsilon}_6+\frac{\vec{\Upsilon}_7+\vec{\Upsilon}_8}{2}\right]^2+\left(\frac{\vec{\Upsilon}_7+\vec{\Upsilon}_8}{2}\right)^2+\Upsilon_7^2+\Upsilon_8^2$$

and so

$$I' = \exp\left[-a\left\{2\left(\vec{\Upsilon}'_2+\frac{\vec{\Upsilon}'_3+\vec{\Upsilon}'_4}{2}\right)^2+\frac{(\vec{\Upsilon}'_3+\vec{\Upsilon}'_4)^2}{2}+\Upsilon_3'^2+\Upsilon_4'^2\right\}\right]$$

$$\exp\left[-a\left\{2\left(\vec{\Upsilon}'_6+\frac{\vec{\Upsilon}_7+\vec{\Upsilon}_8}{2}\right)^2+\left(\frac{\vec{\Upsilon}_7+\vec{\Upsilon}_8}{2}\right)^2+\Upsilon_7'^2+\Upsilon_8'^2\right\}\right]$$

$$\delta\left(\vec{R}-\frac{\vec{R}'}{2}+\frac{\vec{\Upsilon}_4-\vec{\Upsilon}_8}{2}\right) d\vec{\Upsilon}'_2\ldots d\vec{\Upsilon}'_8$$

Now since,

$$\int \exp\left[-\ 2a(\vec{r}+\vec{r}_o)^2\right] d\vec{r} = \int_0^{\pi} \sin\theta\ d\theta \int_0^{2\pi} d\phi \int_0^{\infty} \alpha^2\ \exp -2a\alpha^2 d\alpha = \frac{4\ \pi}{2a^{\frac{3}{2}}}$$

$$\int_0^{\infty} \exp\left[-\ x^2\right] x^2 dx = \left[\frac{\pi}{2a}\right]^{\frac{3}{2}}$$

it follows that

$$I' = \left[\frac{\pi}{2a}\right]^3 \int \exp\left[-\ a\left\{\gamma'^2_3 + \gamma'^2_4 + \left(\frac{\vec{\gamma}'_3 + \vec{\gamma}'_4}{2}\right)^2\right\}\right] \delta\left(\vec{R} - \frac{\vec{R}'}{2} + \frac{\vec{\gamma}'_4 - \vec{\gamma}'_8}{2}\right)\ d\vec{\gamma}'_3 d\vec{\gamma}'_4 d\vec{\gamma}'_7 d\vec{\gamma}'_8$$

Also

$$\gamma^2_3 + \gamma^2_4 + \frac{(\vec{\gamma}_3 + \vec{\gamma}_4)^2}{2} = \frac{3}{2}\ \left(\vec{\gamma}_3 + \frac{\vec{\gamma}_4}{3}\right)^2 + \frac{4\gamma^2_4}{3}$$

Hence

$$I' = \left[\frac{\pi}{2a}\right]^3 \int \exp\left[-\ a\frac{3}{2}\left(\vec{\gamma}'_3 + \frac{\vec{\gamma}'_4}{3}\right)^2 + \frac{4}{3}\ \gamma'^2_4 + \frac{3}{2}\ \left(\vec{\gamma}'_7 + \frac{\vec{\gamma}'_8}{3}\right)^2 + \frac{4}{3}\ \gamma'^2_8\right.$$

$$\delta\left(\vec{R} - \frac{\vec{R}'}{2} + \frac{\vec{\gamma}'_4 - \vec{\gamma}'_8}{2}\right)\ d\vec{\gamma}'_3 d\vec{\gamma}'_4 d\vec{\gamma}'_7 d\vec{\gamma}'_8$$

$$= \left[\frac{\pi}{2a}\right]^3 \left[\frac{\pi 2}{3a}\right]^3 \int \exp\left[-\ \frac{4a}{3}\ (\gamma'^2_4 + \gamma'^2_8)\right] \delta\left(\vec{R} - \frac{\vec{R}'}{2} + \frac{\vec{\gamma}'_4 - \vec{\gamma}'_8}{2}\right)\ d\vec{\gamma}'_4 d\vec{\gamma}'_8$$

Integrating over $\vec{\gamma}'_4$ makes $\vec{\gamma}'_4 = \vec{\gamma}'_8 + \vec{R}' - 2\vec{R}$. Hence

$$I' = \left(\frac{\pi}{a}\right)^6 \times \frac{1}{3^3} \int \exp\left[-\ \frac{4a}{3}\left\{2\vec{\gamma}'^2_8 + 2\ \vec{\gamma}'_8 \cdot (\vec{R}' - 2\vec{R}) + (\vec{R}' - 2\vec{R})^2\right\}\right]\ d\vec{\gamma}'_8$$

But,

$$2\ \gamma^2_8 + 2\vec{\gamma}_8 \cdot (\vec{R}' - 2\vec{R}) + (\vec{R}' - 2\vec{R})^2 = 2(\vec{\gamma}'_8 + \vec{R}' - \vec{R})^2 + \left(\frac{\vec{R}' - 2\vec{R}}{2}\right)^2$$

Hence we obtain the final result

$$I' = \frac{1}{3^3}\ \left(\frac{\pi}{a}\right)^6 \left(\frac{3\pi}{8a}\right)^{\frac{3}{2}} \exp\left[-\ \frac{2a}{3}\ (\vec{R}' - 2\vec{R})^2\right]$$

APPENDIX 16

The object of this appendix is to evaluate the following integral:

$$I'' = \int \exp\left[- a \sum_{i=1}^{8} \gamma_i'^2 \right] \delta\left(\vec{R} - \frac{\vec{\gamma}_7' + \vec{\gamma}_8' - \vec{\gamma}_3' - \vec{\gamma}_4'}{2}\right) d\vec{\gamma}_2' d\vec{\gamma}_3' d\vec{\gamma}_4' d\vec{\gamma}_6' d\vec{\gamma}_8' d{}_7'$$

Comparing this integral with I' in Appendix 15 it follows immediately that:

$$I'' = \left[\frac{\pi}{2a}\right]^3 \int \exp\left[- a\left\{\gamma_3'^2 + \gamma_4'^2 + \frac{(\vec{\gamma}_3' + \vec{\gamma}_4')^2}{2}\right\}\right] \exp\left[- a\left\{\gamma_7'^2 + \gamma_8'^2 + \frac{(\vec{\gamma}_7' + \vec{\gamma}_8')^2}{2}\right\}\right]$$

$$\delta\left(\vec{R} - \frac{\vec{\gamma}_7' + \vec{\gamma}_8' - \vec{\gamma}_3' - \vec{\gamma}_4'}{2}\right) d\vec{\gamma}_3' d\vec{\gamma}_4' d\vec{\gamma}_7' d\vec{\gamma}_8'$$

Next, suppose one integrates over $\vec{\gamma}_3'$. Then, due to the delta function,

$$\vec{\gamma}_3' = \vec{\gamma}_7' + \vec{\gamma}_8' - \vec{\gamma}_4' - 2\vec{R}$$

With a small amount of algebraic manipulation, it then follows that

$$\vec{\gamma}_3'^2 + \vec{\gamma}_4'^2 + \frac{(\vec{\gamma}_3' + \vec{\gamma}_4')^2}{2} = 2\vec{\gamma}_4'^2 - 2\vec{\gamma}_4' \cdot (\vec{\gamma}_7' + \vec{\gamma}_8' - 2\vec{R}) + \frac{3}{2}(\vec{\gamma}_7' + \vec{\gamma}_8' - 2\vec{R})^2$$

From the algebraic identity

$$\vec{\gamma}_4' - \vec{\gamma}_4' \cdot (\vec{\gamma}_7' + \vec{\gamma}_8' - 2\vec{R}) + \frac{3}{4}(\vec{\gamma}_7' + \vec{\gamma}_8' - 2\vec{R})^2 = \left[\vec{\gamma}_4' - \frac{1}{2}(\vec{\gamma}_7' + \vec{\gamma}_8' - 2\vec{R})\right]^2$$

$$+ \frac{1}{2}(\vec{\gamma}_7' + \vec{\gamma}_8' - 2\vec{R})^2$$

It also follows that

$$I'' = \left(\frac{\pi}{2a}\right)^3 \int \exp\left[- 2a\left\{\vec{\gamma}_4' - \frac{1}{2}(\vec{\gamma}_7' + \vec{\gamma}_8' - 2\vec{R})\right\}^2\right] \exp\left[- a\,(\vec{\gamma}_7' + \vec{\gamma}_8' - 2\vec{R})^2\right]$$

$$\exp\left[- a\left\{\vec{\gamma}_7' + \vec{\gamma}_8' + \frac{(\vec{\gamma}_7' + \vec{\gamma}_8')^2}{2}\right\}\right] d\vec{\gamma}_4' d\vec{\gamma}_7' d\vec{\gamma}_8'$$

$$=\left[\frac{\pi}{2a}\right]^{3}\left[\frac{\pi}{2a}\right]^{\frac{3}{2}}\int \exp\left[-\ a(\vec{\Upsilon}'_7+\vec{\Upsilon}'_8-2\vec{R})^2\ -a\left\{\vec{\Upsilon}'_7+\vec{\Upsilon}'_8+\ \frac{(\vec{\Upsilon}'_7+\vec{\Upsilon}'_8)^2}{2}\right\}\right]d\vec{\Upsilon}'_7\,d\vec{\Upsilon}'_8$$

Utilizing the following algebraic identity,

$$(\vec{\Upsilon}'_7+\vec{\Upsilon}'_8-2\vec{R})^2+\vec{\Upsilon}'^2_7+\vec{\Upsilon}'^2_8+\ \frac{(\vec{\Upsilon}'_7+\vec{\Upsilon}'_8)^2}{2}\ =\frac{5}{2}\left[\vec{\Upsilon}'_7-\ \frac{4}{5}\,(\vec{R}-\frac{3\vec{\Upsilon}'_8}{4})\right]^2$$

$$+\ \frac{12}{5}\ (\vec{R}-\frac{\vec{\Upsilon}'_8}{3})^2+\ \frac{4\vec{\Upsilon}'^2_8}{3}$$

the integral becomes

$$I''=\left[\frac{\pi}{2a}\right]^3\left[\frac{\pi}{2a}\right]^{\frac{3}{2}}\left[\frac{2\pi}{5a}\right]^{\frac{3}{2}}\int \exp\left[-\ \frac{12a}{5}\ (\vec{R}-\ \frac{\vec{\Upsilon}'_8}{3})^2\ -\ \frac{4}{3}\,a\vec{\Upsilon}'^2_8\right]d\vec{\Upsilon}'_8$$

$$=\ \exp\left[-\ 2aR^2\right]\left[\frac{\pi}{2a}\right]^3\left[\frac{\pi}{2a}\right]^{\frac{3}{2}}\left[\frac{2\pi}{5a}\right]^{\frac{3}{2}}\int \exp\left[-\ \frac{8a}{5}\,(\vec{\Upsilon}'_8-\ \frac{\vec{R}}{2})^2\ d\vec{\Upsilon}'_8\right.$$

and finally

$$I''=\left[\frac{\pi}{2a}\right]^{\frac{15}{2}}\ \exp\left[-\ 2aR^2\right]$$

APPENDIX 17

The object of this appendix is to evaluate the following integrals:

$$J(p,q,s) = \int R'^{N+2}\, R^{N+2} \exp\left[-pR'^2 + q\vec{R}'\cdot\vec{R} - sR^2\right] Y_\ell^m(\Omega)\, Y_\ell^m(\Omega')^*\, dR\, dR'\, d\Omega\, d\Omega'$$

and

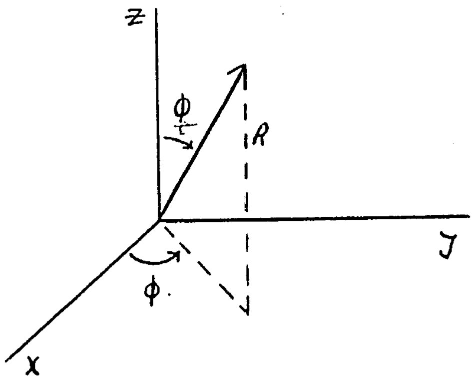
$$Q(p,q,s) = \int R'^{N+2}\, R^{N+3} \exp\left[-pR'^2 + q\vec{R}'\cdot\vec{R} - sR^2\right] Y_\ell^m(\Omega)\, Y_\lambda^m(\Omega')\, dR\, dR'\, d\Omega\, d\Omega'$$

The integration is performed in the (4,0.0), (4,2,0) and (4,4,0) quantum states. (N,ℓ,m) denotes the set of quantum numbers associated with the state.

First, consider the following integral:

$$Q(p,q,s)_{400} = \int R'^6\, R^7 \exp\left[-pR'^2 - sR^2\right] Y_0^0(\Omega)\, dR\, dR'\, d\Omega \int \exp\left[qR'\, R\cos\theta\right] Y_0^0(\Omega')\, d\Omega'$$

where $\vec{R}$ has been fixed along the z-axis while the integration over the primed angles is performed. $Q(p,q,s)_{400}$ denotes $Q(p,q,s)$ with the ground state quantum numbers, $(N,\ell,m) = (4,0,0)$. The coordinate system that is employed is labeled as follows,



But,

$$e^{qR'R\cos\theta'}\, Y_0^0\, (\Omega')^*\, d\Omega' = \int_{-1}^{1} d\mu' \int_0^{2\pi} \frac{\exp}{\sqrt{4\pi}} \left[- \quad qRR'\mu' \quad d\phi \right]$$

$$= \frac{\sqrt{\pi}}{-qRR'} \left\{ \exp\left[-qRR'\right] - \exp\left[qRR'\right] \right\} : q \neq 0$$

Therefore,

$$Q(p,q,s)_{400} = \int_0^{\infty}\int_0^{\infty} R'^6 R^7 \exp\left[-pR'^2 - sR^2\right] \frac{\sqrt{\pi}}{-qRR'} \left\{ \exp\left[-qR'R\right] - \exp\left[qR'R\right.\right.$$

$$dRdR' \int_0^{\pi} d\theta \int_0^{2\pi} d\phi \quad \frac{\sin\theta}{\sqrt{4\pi}} \quad : \quad q \neq 0$$

$$= 2\pi \int_0^{\infty}\int_0^{\infty} \frac{R'^6 R^7 \exp\left[-pR'^2 - sR^2\right]}{-qR'R} \left\{ \exp\left[-qR'R\right] - \exp\left[qR'R\right] \right\} dR'R : q \neq 0$$

Letting $R' = \frac{\omega}{\sqrt{q}}$ and $R = \frac{\nu}{\sqrt{q}}$ the integral becomes

$$Q(p,q,s) = \frac{2\pi}{q^{7+\frac{1}{2}}} \int_0^{\infty} \nu^6 \exp\left[- \frac{s\nu^2}{q} \right] d\nu \int_0^{\infty} \omega^5 \exp\left[- \frac{p\omega^2}{q} \right] \left(e^{\nu\omega} - e^{-\nu\omega} \right) d\omega : q \neq$$

It is easily shown by completing the square in the exponents that

$$\int_0^{\infty} \omega^5 \exp\left[-k\omega^2 \right] \left(e^{\nu\omega} - e^{-\nu\omega} \right) d\omega = \frac{\sqrt{\pi}\, \nu e^{\frac{\nu^2}{4k}}}{8k^{3+\frac{1}{2}}} \left[15 + \frac{5\nu^2}{k} + \frac{\nu^4}{4k^2} \right]$$

Therefore

$$Q(p,q,s)_{400} = \frac{\pi^{\frac{3}{2}}}{4q^{\frac{15}{2}}\, k^{\frac{7}{2}}} \int_0^{\infty} \nu^7 \exp\left[-\left(\frac{s}{q} - \frac{q}{4p} \right) \nu^2 \right] \left[15 + \frac{5\nu^2}{k} + \frac{\nu^4}{4k^2} \right] d\nu : q \neq$$

where $k = \frac{p}{q}$

And because,

$$\int_0^\infty x^{2N+1} \exp\left[-kx^2\right] dx = \frac{N!}{2k^{N+1}}$$

it follows that

$$Q(p,q,p)_{400} = \frac{\pi^{\frac{3}{2}}\, 5!}{8q^4 p^{\frac{7}{2}} \left(\frac{p}{q} - \frac{q}{4p}\right)^4} \left[\frac{3}{4} + \frac{q}{p\left(\frac{p}{q} - \frac{q}{4p}\right)} + \frac{q^2}{4p^2 \left(\frac{p}{q} - \frac{q}{4p}\right)^2}\right] : q \neq 0$$

It follows from the orthogonality property of the spherical harmonic functions that

$$Q(p,q,p)_{420} = Q(p,q,p)_{440} = 0$$

It is clear from the preceding work that

$$J(p,q,p)_{400} = \frac{\pi^{\frac{3}{2}}}{4q^{\frac{7}{2}} p^{\frac{7}{2}}} \int_0^\infty \nu^6 \exp\left[-\left(\frac{p}{q} - \frac{q}{4p}\right)\nu^2\right]\left[15 + \frac{5q\nu^2}{p} + \frac{q^2\nu^4}{4p^2}\right] d\nu \qquad q \neq 0$$

It then follows from

$$\int_0^\infty x^{2N} \exp\left[-kx^2\right] dx = \frac{1\cdot3\cdot5\ldots(2N-1)}{2^{N+1}\, k^N}\sqrt{\frac{\pi}{k}}$$

that

$$J(p,q,p)_{400} = \frac{15\,\pi^2}{2^6 q^{\frac{7}{2}} p^{\frac{7}{2}} \left(\frac{p}{q} - \frac{q}{4p}\right)^{3+\frac{1}{2}}} \left[15 + \frac{35q}{2p\left(\frac{p}{q} - \frac{q}{4p}\right)} + \frac{9\cdot7\, q^2}{2^4 p^2 \left(\frac{p}{q} - \frac{q}{4p}\right)^2}\right]; q \neq$$

Once again it follows from the orthogonality property of the spherical harmonic functions that

$$J(p,q,p)_{420} = J(p,q,p)_{440} = 0 \; : \; q \neq 0$$

Now consider the integration involved in $Q(p,0,s)$; in particular consider:

$$Q(p,0,s)_{400} = \int R'^{6} \, R^{7} \exp\left[-pR'^{2} - sR^{2}\right] dR \, dR' \int Y_{o}^{o}(\Omega)\, d\Omega \int Y_{o}^{o}(\Omega')\, d\Omega'$$

This reduces to:

$$Q(p,0,s)_{400} = 4\pi \int_{0}^{\infty} R^{7} \exp\left[-sR^{2}\right] dR \int_{0}^{\infty} R'^{6} \exp\left[-pR'^{2}\right] dR'$$

By letting $R' = \dfrac{\omega}{\sqrt{p}}$ and $R = \dfrac{\nu}{\sqrt{s}}$, this becomes:

$$Q(p,0,s)_{400} = \frac{4\pi}{s^{4}\, p^{\frac{7}{2}}} \int_{0}^{\infty} \nu^{7} \exp\left[-\nu^{2}\right] d\nu \int_{0}^{\infty} \omega^{6} \exp\left[-\omega^{2}\right] d\omega$$

$$= \frac{5 \cdot 3\, \pi^{\frac{3}{2}}}{4s^{4}\, p^{\frac{7}{2}}} \int_{0}^{\infty} \nu^{7} \exp\left[-\nu^{2}\right] d\nu$$

which reduces to:

$$Q(p,0,s)_{400} = \frac{5 \cdot 3^{2}\, \pi^{\frac{3}{2}}}{4s^{4}\, p^{\frac{7}{2}}}$$

and finally:

$$Q(p,0,p)_{400} = \frac{5 \cdot 3^{2}\, \pi^{\frac{3}{2}}}{4p^{7+\frac{1}{2}}}$$

From the orthogonality property of the spherical harmonic functions it again follows that:

$$Q(p,0,p)_{420} = Q(p,0,p)_{440} = 0$$

Also it is seen immediately that:

$$J(p,0,s)_{400} = \frac{5\cdot 3\, \pi^{\frac{3}{2}}\sqrt{s}}{4s^4\, p^{\frac{7}{2}}} \int_0^{\infty} \nu^6 \exp\left[-\, \nu^2\right] d\nu = \frac{15^2\, \pi^2\, \sqrt{s}}{2^6\, s^4\, p^{\frac{7}{2}}}$$

and:

$$J(p,0,p)_{400} = \frac{15^2\, \pi^2}{2^6\, p^7}$$

and as a consequence of the orthogonality property of the spherical harmonic functions involved

$$J(p,0,p)_{420} = J(p,0,p)_{440} = 0$$

APPENDIX 18

The object of this appendix is to evaluate the following integral:

$$\mathcal{Q}(p,q,s)_{N\ell m} = \int R'^{N+2}\, R^{N+4} \exp\left[-pR'^2 + q\vec{R'}\cdot\vec{R} - sR^2\right] Y_\ell^m(\Omega)\, Y_\ell^m(\Omega')\; dR\, dR'\, d\Omega\, d\Omega'$$

First consider the following integral:

$$\mathcal{Q}(p,q,s)_{400} = \int R'^6\, R^8 \exp\left[-pR'^2 - sR^2\right] Y_0^0(\Omega)\, dR\, dR'\, d\Omega \int e^{qR'R\cos\theta'}\, Y_0^0(\Omega')\, d\Omega'$$

where $\vec{R}$ has been fixed along the z-axis while the integration over the primed angles is performed. It now follows from Appendix 17 that:

$$\mathcal{Q}(p,q,p)_{400} = \frac{\pi^{\frac{3}{2}}}{4q^8\, k^{\frac{7}{2}}} \int_0^\infty \nu^8 \exp\left[-\left(\frac{p}{q} - \frac{q}{4p}\right)\nu^2\right] \left[15 + \frac{5\nu^2}{k} + \frac{\nu^4}{4k^2}\right] d\nu \qquad \left(k = \frac{p}{q}\right)$$

and because:

$$\int_0^\infty x^{2n} \exp\left[-\alpha x^2\right] dx = \frac{1\cdot 3\cdot 5\ldots(2n-1)\sqrt{\pi}}{2^{n+1}\, \alpha^{n+\frac{1}{2}}}$$

$$\mathcal{Q}(p,q,p)_{400} = \frac{\pi^2\; 7\cdot 5\cdot 3^2}{2^7 q^{\frac{9}{2}} p^{\frac{7}{2}} \left(\frac{p}{q} - \frac{q}{4p}\right)^{4+\frac{1}{2}}} \left[5 + \frac{5\cdot 3q}{2p\left(\frac{p}{q} - \frac{q}{4p}\right)} + \frac{11\cdot 3\, q^2}{2^4 p^2 \left(\frac{p}{q} - \frac{q}{4p}\right)^2}\right] : q \neq 0$$

It follows from the orthogonality property of the spherical harmonic functions that:

$$\mathcal{L}(p,q,p)_{420} = \mathcal{L}(p,q,p)_{440} = 0 \quad : \quad q \neq 0$$

Now consider the integrations involved in $\mathcal{L}(p,0,s)_{N\ell m}$ and in particular consider

$$\mathcal{L}(p,0,s)_{400} = \int R'^{6} R^{8} \exp\left[-pR'^{2} - sR^{2}\right] dR\,dR' \int Y^{o}_{o}(\Omega)\,d\Omega \int Y^{o}_{o}(\Omega')\,d\Omega'$$

It follows from Appendix 17 that:

$$\mathcal{L}(p,0,s)_{400} = \frac{5 \cdot 3\,\pi^{\frac{3}{2}}}{4s^{4+\frac{1}{2}}\,p^{3+\frac{1}{2}}} \int_{0}^{\infty} \nu^{8} \exp\left[-\nu^{2}\right] d\nu$$

and so:

$$\mathcal{L}(p,0,p)_{400} = \frac{5^{2} \cdot 3^{2} \cdot 7\,\pi^{2}}{2^{7} p^{8}}$$

and again due to the orthogonality property of the spherical harmonics:

$$\mathcal{L}(p,0,p)_{420} = \mathcal{L}(p,0,p)_{440} = 0$$

APPENDIX 19

The object of this appendix is to evaluate the following integral:

$$I_7 = \int \Upsilon_8^2 \exp\left[-a\sum_{i=1}^{8}\Upsilon_i^2\right] R^{2N} \exp\left[-2\beta R^2\right] Y_\ell^m(\Omega)^* \, Y_\ell^m(\Omega)\, d\tau$$

Since the spherical harmonic functions used in the above equation are normalized and also N=4 for the ground state and first two excited states, it follows that:

$$I_7 = \frac{2^{15}\cdot 9\cdot 7\cdot 5\cdot 3\sqrt{\pi}}{2^{11+\frac{1}{2}}\,\beta^{5+\frac{1}{2}}} \int \Upsilon_8^2 \exp\left[-a\sum_{i=1}^{8}\Upsilon_i^2\right] d\vec{\Upsilon}_2\, d\vec{\Upsilon}_3\, d\vec{\Upsilon}_4\, d\vec{\Upsilon}_6\, d\vec{\Upsilon}_7\, d\vec{\Upsilon}_8$$

From Appendix 15 it follows that:

$$\int \Upsilon_8^2 \exp\left[-a\sum_{i=1}^{8}\Upsilon_i^2\right] d\vec{\Upsilon}_2\, d\vec{\Upsilon}_3\, d\vec{\Upsilon}_4\, d\vec{\Upsilon}_6\, d\vec{\Upsilon}_7\, d\vec{\Upsilon}_8 = \frac{\pi^6}{3^3\, a^6} \int \Upsilon_8^2 \exp\left[-\frac{4a}{3}\left(\Upsilon_4^2 + \Upsilon_8^2\right)\right] d\vec{\Upsilon}_4\, d\vec{\Upsilon}_8$$

$$= \frac{3^2\,\pi^9}{2^9\cdot a^{10}}$$

Therefore:

$$I_7 = \frac{3^5\cdot 7\cdot 5\;\pi^{9+\frac{1}{2}}}{2^{5+\frac{1}{2}}\;\epsilon^{5+\frac{1}{2}}\;a^{15+\frac{1}{2}}}$$

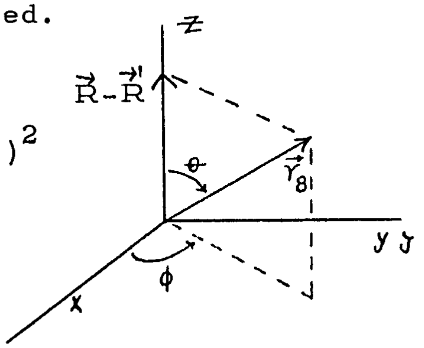
It is seen that the result is the same for the ground state and the first two excited states.

APPENDIX 20

In this appendix the following integral is evaluated:

$$I = \int \gamma_8^2 \exp\left[-\frac{8a}{3} (\vec{\gamma}_8 + \vec{R} - \vec{R}')^2\right] d\vec{\gamma}_8$$

The direction of $\vec{R} - \vec{R}'$ is fixed along the direction of the z-axis while the integration is performed.



Then

$$(\vec{\gamma}_8+\vec{R}-\vec{R}')^2 = \gamma_8^2 + 2\gamma_8|\vec{R}-\vec{R}'| \cos\theta + (R-R')^2$$

Therefore

$$I = \int_0^\infty \gamma_8^4 \exp\left[-\frac{8a}{3} (\gamma_8^2 + (\vec{R}-\vec{R}')^2\right] d\gamma_8 \int_0^\pi \exp\left[-\frac{16a}{3} |\vec{R}-\vec{R}'| \gamma_8 \cos\theta\right] \sin\theta \, d\theta \int_0^{2\pi} d\phi$$

$$= \frac{3\pi}{|\vec{R}-\vec{R}'| \cdot 8a} \int_0^\infty \gamma_8^3 \left\{\exp\left[-\frac{8a}{3} (\gamma_8 - |\vec{R}+\vec{R}'|)^2\right] - \exp\left[-\frac{8a}{3}(\gamma_8 + |\vec{R}-\vec{R}'|)^2\right\}\right] d\gamma_8$$

$$= \frac{3\pi}{8a|\vec{R}-\vec{R}'|} \int_0^\infty \exp\left[-\frac{8a}{3} \alpha^2\right]\left[(\alpha+|\vec{R}-\vec{R}'|)^3 - (\alpha-|\vec{R}-\vec{R}'|)^3\right] d\alpha$$

$$= \frac{3^{\frac{3}{2}} \pi^{\frac{3}{2}}}{a^{2+\frac{1}{2}} \, 2^{8+\frac{1}{2}}} \left[3^2 + 2^4 (\sqrt{a}\vec{R} - \sqrt{a}\vec{R}')^2 \right]$$

APPENDIX 21

The object of this Appendix is to evaluate the following integral

$$T(p,q,p)_{400} = \int R^6 R'^6 \exp\left[-pR^2 + 2\vec{R}\cdot\vec{R}' - pR'^2\right] Y_0^0(\Omega) Y_0^0(\Omega')\vec{R}\cdot\vec{R}'\,dR\,dR'\,d\Omega\,d\Omega'$$

Keeping the direction of $\vec{R}$ fixed along the z-axis and integrating over all directions of $\vec{R}'$ the integral becomes

$$T(p,q,p) = 2\pi \int R^7 R'^7 \exp -pR^2 - pR'^2 \quad dR\,dR' \int_0^{\pi} e^{qRR'\cos\theta'} \cos\theta' \sin\theta' d\theta'$$

$$= \frac{2\pi}{q^8}\left[T_1 + T_2\right]$$

where

$$T_1 = \int_0^{\infty} x^6 e^{-kx^2} dx \int_0^{\infty} w^6 e^{-kw^2} (e^{xw} + e^{-xw}) dw$$

$$T_2 = -\int_0^{\infty} x^5 e^{-kx^2} dx \int_0^{\infty} w^5 e^{-kw^2} (e^{xw} - e^{-xw}) dw$$

and $k = \frac{p}{q}$

Performing these integrations one obtains

$$T_1 = \frac{5^2 \cdot 3^2 \pi}{(4k^2 - 1)^{3+\frac{1}{2}}} \left[1 + \frac{7\cdot 3}{(4k^2 - 1)} + \frac{3^2 \cdot 7}{(4k^2 - 1)^2} + \frac{11\cdot 7\cdot 3}{5(4k^2 - 1)^3} \right]$$

$$T_2 = -\frac{5^2 \cdot 3^2 \pi}{(4k^2 - 1)^{3+\frac{1}{2}}} \left[1 + \frac{7\cdot 2}{3(4k^2 - 1)} + \frac{7\cdot 3}{5(4k^2 - 1)^2} \right]$$

and finally

$$T(p,q,p) = \frac{7^2 \cdot 5^2 \cdot 3 \cdot 2^2 \pi}{q^8 (4k^2 - 1)^{4+\frac{1}{2}}} \left[1 + \frac{3^2 \cdot 2}{5(4k^2 - 1)} + \frac{11\cdot 3^2}{7\cdot 5(4k^2 - 1)^2} \right]$$

APPENDIX 22

In this appendix the following integral is evaluated:

$$I_8 = \int \psi(48)^* \; \gamma_8^2 \; \psi(o) \; d\tau$$

Writing the explicit expression for I_8 out, we have:

$$I_8 = 2^{15} \int \gamma_8^2 \; \exp\left[- \frac{a}{2} \sum_{i=1}^{8} \gamma_i^2 \right] R^N \; \exp\left[-\beta R^2 \right] Y_l^m(\Omega) \; d\vec{\gamma}_2 \ldots d\vec{\gamma}_8 d\vec{R}$$

$$\int \exp\left[- \frac{a}{2} \sum_{i=1}^{8} \gamma_i'^2 \right] R'^N \; \exp\left[-\beta R'^2 \right] Y_l^m(\Omega)^* \;\; \delta(\vec{r}_1-\vec{r}'_1)\, \delta(\vec{r}_2-\vec{r}'_2)\, \delta(\vec{r}_3-\vec{r}'_3)$$

$$\delta(\vec{r}_8-\vec{r}'_4)\, \delta(\vec{r}_5-\vec{r}'_5)\, \delta(\vec{r}_6-\vec{r}'_6)\, \delta(\vec{r}_7-\vec{r}'_7)\, \delta(\vec{r}_4-\vec{r}'_8) \;\; d\tau'$$

The delta functions in this equation cause the following relationship between the primed and unprimed independent particle coordinates:

$\vec{r}_1=\vec{r}'_1$, $\vec{r}_2=\vec{r}'_2$, $\vec{r}_3=\vec{r}'_3$, $\vec{r}_4=\vec{r}'_8$, $\vec{r}_5=\vec{r}'_5$, $\vec{r}_6=\vec{r}'_6$, $\vec{r}_7=\vec{r}'_7$, $\vec{r}_8=\vec{r}'_4$

It is seen that in the cluster system of coordinates one of the delta functions can be written as $\delta(\vec{R}_{cm}-\vec{R}'_{cm})$. The above relationship between the primed and unprimed independent particle coordinate systems causes the following relationship between the primed and unprimed coordinates in the cluster systems of coordinates.

$$\vec{R}' = \frac{\vec{R}}{2} - \frac{\vec{\gamma}_4 - \vec{\gamma}_8}{2}$$

Hence another delta function in the cluster coordinate system is

$\delta(\vec{R}' - \frac{\vec{R}}{2} + \frac{\vec{\gamma}_4 - \vec{\gamma}_8}{2})$. Suppose we now integrate over the primed internal coordinates. This integration is equivalent to replacing the left hand side of the equation:

$$\sum_{i=1}^{8} \gamma_i'^2 = \sum_{i=1}^{8} \gamma_i^2 - 2(R'^2 - R^2)$$

by the right hand side. Therefore we have:

$$I_8 = 2^{15} \int \gamma_8^2 \exp\left[-a \sum_{i=1}^{8} \gamma_i^2 + a(R'^2 - R^2)\right] R^N \exp\left[-\beta R^2\right] Y_\ell^m(\Omega) R'^N$$

$$\exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')^* \, \delta(\vec{R}' - \frac{\vec{R}}{2} + \frac{\vec{\gamma}_4 - \vec{\gamma}_8}{2}) \, d\vec{\gamma}_2 d\vec{\gamma}_3 d\vec{\gamma}_4 d\vec{\gamma}_6 d\vec{\gamma}_7 d\vec{\gamma}_8 \, d\vec{R} \, d\vec{R}'$$

It follows from Appendix 15 that:

$$\int \gamma_8^2 \exp\left[-a \sum_{i=1}^{8} \gamma_i^2\right] \delta(\vec{R}' - \frac{\vec{R}}{2} + \frac{\vec{\gamma}_4 - \vec{\gamma}_8}{2}) \, d\vec{\gamma}_2 d\vec{\gamma}_3 d\vec{\gamma}_4 d\vec{\gamma}_6 d\vec{\gamma}_7 d\vec{\gamma}_8$$

$$= \frac{\pi^6}{3^3 a^6} \exp\left[-\frac{2a}{3} (\vec{R} - 2\vec{R}')^2\right] \int \gamma_8^2 \exp\left[-\frac{8a}{3} (\vec{\gamma}_8 + \vec{R} - \vec{R}')^2\right] d\vec{\gamma}_8$$

Also it is shown in Appendix 20 that

$$\int \gamma_8^2 \exp\left[-\frac{8a}{3} (\vec{\gamma}_8 + \vec{R} - \vec{R}')^2\right] d\vec{\gamma}_8 = \frac{3^{\frac{3}{2}} \pi^{\frac{3}{2}}}{a^{2+\frac{1}{2}} \, 2^{8+\frac{1}{2}}} \left[3^2 + 2^4 (\sqrt{a}\vec{R} - \sqrt{a}\vec{R}')^2\right]$$

Therefore

$$I_8 = \frac{2^{6+\frac{1}{2}} \pi^{7+\frac{1}{2}}}{3^{\frac{3}{2}} a^{8+\frac{1}{2}}} \int \exp\left[-(\frac{5a}{3} + \beta) R^2 + \frac{8a}{3} \vec{R} \cdot \vec{R}' - (\frac{5a}{3} + \beta) R'^2\right] R^4 R'^4$$

$$\left[3^2 + 2^4 (\sqrt{a}\vec{R} - \sqrt{a}\vec{R}')^2\right] Y_\ell^m(\Omega) Y_\ell^m(\Omega')^* \, d\vec{R} \, d\vec{R}'$$

At this point it is clear that I_8 is zero in the excited states and it is also clear that for the complete integration in the ground state

$$I_8 = \frac{2^{6+\frac{1}{2}}\,\pi^{7+\frac{1}{2}}\,3^{\frac{1}{2}}}{a^{8+\frac{1}{2}}} \left[J(p,q,p)_{400} + \frac{2^5 a}{3^2}\mathcal{L}(p,q,p)_{400} - \frac{2^5 a}{3^2} T(p,q,p)_{400} \right]$$

where

$$p = \frac{5a}{3} + \beta \quad , \qquad q = \frac{8a}{3}$$

and $T(p,q,p)$ is defined in Appendix 21.

APPENDIX 23

The object of this appendix is to evaluate the following integral:

$$I = \int \gamma_8^2 \exp\left[- \frac{8a}{5} \left(\vec{\gamma}_8 - \frac{\vec{R}'}{2} \right) \right] d\vec{\gamma}_8$$

First the direction of $\vec{R}'$ is fixed along the z-axis and the integration over the various directions of $\vec{\gamma}_8$ is performed.

$$I = \exp\left[- \frac{2aR'^2}{5} \right] \int_0^\infty \gamma_8^4 \exp\left[- \frac{8a\gamma_8^2}{5} \right] d\gamma_8 \int_0^{2\pi} d\phi \int_0^\pi \exp\left[+ \frac{8a}{5} \gamma_8 R' \cos\theta \right] \sin\theta \, d\theta$$

$$= \frac{5\pi}{4aR'} \int_0^\infty \gamma_8^3 \left\{ \exp\left[- \frac{8a}{5} \left(\gamma_8 - \frac{R'}{2} \right)^2 \right] - \exp\left[\frac{8a}{5} \left(\gamma_8 + \frac{R'}{2} \right)^2 \right] \right\} d\gamma_8$$

$$= \frac{5\pi}{4aR'} \int_0^\infty \exp\left[- \frac{8ax^2}{5} \right] \left(3R'x^2 + \frac{R'^3}{4} \right) dx$$

$$= \frac{5^{\frac{3}{2}} \pi^{\frac{3}{2}}}{2^{6+\frac{1}{2}} a^{2+\frac{1}{2}}} \left[\frac{5 \cdot 3}{2^2} + \left(\sqrt{a} R' \right)^2 \right]$$

APPENDIX 24

The object of this appendix is to evaluate the following integral:

$$I_9 = \int \psi(37,48)^* \, \gamma_8^2 \, \psi(o) \, d\tau$$

in the ground state and the first two excited states.

I_9 can be written down explicitly as follows,

$$I_9 = 2^{15} \int \gamma_8^2 \exp\left[-\frac{a}{2} \sum_{i=1}^{8} \gamma_i^2\right] R^N \exp\left[-\beta R^2\right] Y_\ell^m(\Omega) \, d\vec{\gamma}_2 \, d\vec{\gamma}_3 \, d\vec{\gamma}_4 \, d\vec{\gamma}_6 \, d\vec{\gamma}_7 \, d\vec{\gamma}_8 \, d\vec{R}$$

$$\int \exp\left[-\frac{a}{2} \sum_{i=1}^{8} \gamma_i'^2\right] R'^N \exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')^* \, \delta(\vec{r}_1 - \vec{r}_1') \, \delta(\vec{r}_2 - \vec{r}_2')$$

$$\delta(\vec{r}_7 - \vec{r}_3') \, \delta(\vec{r}_8 - \vec{r}_4') \quad \delta(\vec{r}_r - \vec{r}_5') \, \delta(\vec{r}_6 - \vec{r}_6') \, \delta(\vec{r}_3 - \vec{r}_7') \, \delta(\vec{r}_4 - \vec{r}_8') \, d\tau'$$

The following relationship between the primed and unprimed independent particle coordinates is caused by the delta functions in the above expression:

$$\vec{r}_1 = \vec{r}_1', \quad \vec{r}_2 = \vec{r}_2', \quad \vec{r}_3 = \vec{r}_7', \quad \vec{r}_4 = \vec{r}_8', \quad \vec{r}_5 = \vec{r}_5', \quad \vec{r}_6 = \vec{r}_6', \quad \vec{r}_7 = \vec{r}_3', \quad \vec{r}_8 = \vec{r}_4$$

It is immediately clear that in the cluster system of coordinates one of the delta functions can be written as $\delta(\vec{R}_{cm} - \vec{R}_{cm}')$. Also the relationship

$$\vec{R}' = \frac{\vec{\gamma}_7 + \vec{\gamma}_8 - \vec{\gamma}_3 - \vec{\gamma}_4}{2}$$

is an immediate consequence of the relationship between the primed and unprimed independent particle system of coordinates. Thus another delta function in the cluster coordinate system is

$$\delta(\vec{R}' - \frac{\vec{\gamma}_7 + \vec{\gamma}_8 - \vec{\gamma}_3 - \vec{\gamma}_4}{2}).$$

It is now seen that an integration over the primed internal coordinates is equivalent to replacing the left hand side of the equation

$$\sum_{i=1}^{8} \gamma_i'^2 = \sum_{i=1}^{8} \gamma_i^2 - 2(R'^2 - R^2)$$

by the right hand side. The integral denoted by I_9 now becomes;

$$I_9 = 2^{15} \int \gamma_8^2 \exp\left[-a \sum_{i=1}^{8} \gamma_i^2 + a(R'^2 - R^2)\right] R^N \exp\left[-\beta R^2\right] Y_\ell^m(\Omega)\ R'^N \exp\left[-\beta R'^2\right] Y_\ell^m(\Omega')^* \ \delta(\vec{R}' - \frac{\vec{\gamma}_7 + \vec{\gamma}_8 - \vec{\gamma}_3 - \vec{\gamma}_4}{2})\ d\vec{\gamma}_2 d\vec{\gamma}_3 d\vec{\gamma}_4 d\vec{\gamma}_6 d\vec{\gamma}_7 d\vec{\gamma}_8\ d\vec{R}\ d\vec{R}'$$

From Appendix 16 it is seen that:

$$\int \gamma_8^2 \exp\left[-a \sum_{i=1}^{8} \gamma_i^2\right] \delta(\vec{R}' - \frac{\vec{\gamma}_7 + \vec{\gamma}_8 - \vec{\gamma}_3 - \vec{\gamma}_4}{2})\ d\vec{\gamma}_2 d\vec{\gamma}_3 d\vec{\gamma}_4 d\vec{\gamma}_6 d\vec{\gamma}_7 d\vec{\gamma}_8$$

$$= \frac{\pi^6}{2^3 a^6} \exp\left[-2aR'^2\right] \int \gamma_8^2 \exp\left[-\frac{8a}{5}(\vec{\gamma}_8 - \frac{\vec{R}'}{2})\right] d\vec{\gamma}_8$$

In Appendix 23 it is shown that

$$\int \gamma_8^2 \exp\left[-\frac{8a}{5}(\vec{\gamma}_8 - \frac{\vec{R}'}{2})\right] d\vec{\gamma}_8 = \frac{5^{\frac{3}{2}} \pi^{\frac{3}{2}}}{a^{2+\frac{1}{2}}\ 2^{6+\frac{1}{2}}} \left[\frac{3\cdot 5}{2^2} + (\sqrt{a}R')^2\right]$$

Therefore

$$I_9 = \frac{2^{5+\frac{1}{2}} \pi^{7+\frac{1}{2}}}{a^{8+\frac{1}{2}}} \cdot \Bigg[\frac{5\cdot 3}{2^2} \int R^N \exp\left[-(a+\beta)R^2\right] R'^N \exp\Big[-(a+\beta)R'^2\ Y_\ell^m(\Omega)\ Y_\ell^m(\Omega')^* d\vec{R} d\vec{R}'$$

$$+ \; a \int R^{N} \exp\left[-(a+\beta)R^{2}\right] R'^{\,N+2} \exp\left[-(a+\beta)R^{2}\right] Y_{\ell}^{m}(\Omega) \; Y_{\ell}^{m}(\Omega')^{*} d\vec{R} d\vec{R}' \Bigg]$$

$$= \frac{2^{5+\frac{1}{2}} \; \pi^{7+\frac{1}{2}}}{a^{8+\frac{1}{2}}} \left[\frac{5 \cdot 3}{2^{2}} \; J(a+\beta, 0, a+\beta) \; + \; a \, \lambda(a+\beta, 0, a+\beta) \right]$$

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