THE α-PARTICLE MODEL OF O^{16}

Thesis by

Stanley L. Kameny

In Partial Fulfillment of the Requirements
for the Degree of
Doctor of Philosophy

California Institute of Technology
Pasadena, California
1955

ACKNOWLEDGMENTS

It gives me great pleasure to thank Professor Robert F. Christy for suggesting the problem and for his encouragement and helpful advice.

I should like also to thank Dr. Donald L. Drukey for providing a needed prod and an open ear during the early stages of the work, and Miss Rosemarie Stampfel for her care and patience in preparing the typescript.

ABSTRACT

The α-particle model is re-derived and used to calculate the energy levels of O^{16}, extending the work of Dennison to include all levels up to 15 Mev.

Wave functions for low lying levels are used to compute the lifetimes of the first four excited levels of O^{16}.

In addition, the model is applied to furnish core wave functions for a partially-excited-core shell model of O^{17}. The lifetime of the 870 Kev level and the electric quadrupole and magnetic moments of the ground state are computed.

The energy level predictions are found to be in good agreement with experiment, but the lifetime predictions are only fair. The O^{17} model can provide quantitative agreement with the lifetime only.

The evidence favoring either of the two identification schemes proposed by Dennison is not conclusive.

TABLE OF CONTENTS

TABLE OF CONTENTS (cont.)

TABLE OF CONTENTS (cont.)

PART I. GENERAL CONSIDERATIONS

1. The α-particle Model.

The α-particle model of O^{16} assumes the nucleus to be a semi-rigid structure of four α-particles, held together by mutual attraction and repulsion. The model regards the excited states as the result of rotations and/or normal vibrations of the structure, consistent with the requirement that the wave function be symmetric in all four α-particles. Except perhaps for the severe symmetry requirement (which restricts the number of available states) the model resembles the usual molecular models [1]. For purposes of calculation, one neglects the actual form of the forces involved, and considers the particles to be harmonically bound to an equilibrium configuration. The vibrations involved are assumed to be of small amplitude so that the structure is unchanged in the large, and deviations of the potential from the harmonic are treated as perturbations.

One has several different approaches in handling the model. One could, for example, use knowledge of forces obtained from α-α scattering experiments to deduce the energy levels. Another approach, which will be used here, is to determine the effective constants such as the equilibrium separation and the force constants, from the energy levels, and make predictions of lifetimes, etc. from these. Thus lifetimes will be given as functions of energy levels, with the model furnishing the connecting structure. Actually, the inductive procedure is far safer than the deductive approach, since it makes no assumption that the effective forces among a group of α-particles are the sum of pair forces, and allows for the possibility of 3 and 4-body forces.

2.0. The Hamiltonian.

The classical Hamiltonian for a semi-rigid rotation has been derived by Wilson and Howard [2]. The correct transition to the quantum mechanical form of the semi-rigid rotator Hamiltonian is difficult to find in the literature.* Although the differences between the correct Hamiltonian and the various incorrect forms are present only in terms which we will neglect in the approximations which we shall employ here, we include a rederivation of the Hamiltonian both for completeness and to resolve the confusion.

2.1. Classical Hamiltonian.

Consider a set of N particles m with masses m_m and cartesian coordinates $\vec{x}_m$.

The kinetic energy is $T = \frac{1}{2} \sum_{m=1}^{N} m_m \dot{\vec{x}}_m \cdot \dot{\vec{x}}_m$.

To eliminate the motion of the center of mass, define

$$M = \sum_{m=1}^{N} m_m$$

$$\vec{X} = \frac{1}{M} \sum_{m=1}^{N} m_m \vec{x}_m$$

$$\vec{r}_m = \vec{x}_m - \vec{X} \quad .$$

Then

$$T = \frac{1}{2} M \dot{X}^2 + \frac{1}{2} \sum_{m=1}^{N} m_m \dot{\vec{r}}_m \cdot \dot{\vec{r}}_m \quad .$$

Let there be a potential $V(\vec{x}_m)$ which is independent of the position of the center of mass, so that

$$V(\vec{x}_m) = V_r(\vec{r}_m) \quad .$$

---

* Compare, for example, the Q.M. Hamiltonian given in ref. [3] with the correct form given in ref. [4].

Further, let the potential be invariant under rotation of the entire configuration, so that, if $\tilde{R}(\theta)$ (the notation ~ signifies a dyadic) represents a rotation of coordinates $\vec{s}_m$ to $\vec{r}_m$, such that

$$\vec{r}_m = \tilde{R}(\theta) \cdot \vec{s}_m \,, \quad \text{then}$$

$$V_r(\vec{r}_m) = V_s(\vec{s}_m) \quad \text{for all} \quad \tilde{R}(\theta) \,.$$

Lastly, let there be an equilibrium configuration designated by $\vec{a}_m$, and let $\vec{\rho}_m$ designate deviations from the equilibrium position, such that

$$\vec{s}_m = \vec{a}_m + \vec{\rho}_m$$

and $V_s(\vec{s}_m) = V_o + V_\rho(\vec{\rho}_m)$ where $V_\rho(\vec{\rho}_m)$ is composed of terms of second and higher orders in the components of $\vec{\rho}_m$ and satisfies the conditions that $\vec{\rho}_m = 0$ is a true minimum.

$$V = V_o + \sum_{mn} \vec{\rho}_m \cdot \tilde{V}_{mn} \cdot \vec{\rho}_n + \text{(higher orders).}$$

Now in order to transform the kinetic energy, consider a small variation $\delta \vec{r}_m$ in the positions of particles. For the transformation into rotational coordinates $\vec{\theta}$ and vibrational coordinates $\vec{\rho}_m$ to be valid, we must be able to express any arbitrary variation $\delta \vec{r}_m$ (consistent with $\sum_m m_m \delta \vec{r}_m = 0$) uniquely in terms of an infinitesimal rotation $\delta\vec{\theta}$ and an infinitesimal distortion $\delta\vec{\rho}_m$.

We have

$$\delta\vec{r}_m = (\delta\tilde{R}(\theta)) \cdot (\vec{s}_m) + \tilde{R}\cdot(\delta\vec{\rho}_m) \,,$$

but

$$\delta\tilde{R} \cdot = \tilde{R}(\theta) \cdot \delta\vec{\theta} \, x$$

or

$$\delta \vec{r}_m = \tilde{R}(\theta) \cdot (\delta \vec{\theta} \times \vec{s}_m + \delta \vec{\rho}_m) ,$$

and the condition of validity will be that this relation can be solved for $\delta \vec{\theta}$.*

Using the inverse rotation $\tilde{R}^{-1}(\theta)$, we get

$$\tilde{R}^{-1}(\theta) \cdot \delta \vec{r}_m = \delta \vec{\theta} \times \vec{s}_m + \delta \vec{\rho}_m \quad .$$

We form

$$\sum_{m=1}^{N} m_m \vec{a}_m \times \tilde{R}^{-1}(\theta) \cdot \delta \vec{r}_m = \sum_{m=1}^{N} m_m \vec{a}_m \times \delta \vec{\rho}_m + \sum_{m=1}^{N} m_m [\vec{a}_m \times (\delta \vec{\theta} \times \vec{s}_m)]$$

and note that of the $\delta \vec{r}_m$, only $3N - 3$ components are independent since $\sum_{m=1}^{N} m_m \vec{r}_m = 0$. If in addition we are to obtain the $\delta \vec{\theta}$ as three independent variations, then only $3N - 6$ of the components of $\delta \vec{\rho}_m$ can be independent, hence we are at liberty to fix three linear relations among the $\vec{\rho}_m$, in particular, to require that

$$\sum_{m=1}^{N} m_m \vec{a}_m \times \vec{\rho}_m = 0 \quad .$$

We are then left with

$$\sum_{m=1}^{n} m_n \vec{a}_m \times \tilde{R}^{-1}(\theta) \cdot \delta \vec{r}_m = \delta \vec{\theta} \cdot \tilde{B}(\vec{\rho}_m)$$

where

$$\tilde{B}(\vec{\rho}_m) = \sum_{m=1}^{N} m_m [\tilde{1}(\vec{a}_m \cdot \vec{s}_m) - \vec{a}_m \vec{s}_m];$$

$\tilde{1}$ = unit dyad; $\vec{a}_m \vec{s}_m$ = outer product.

---

* This is the same as the requirement that the Jacobian $\dfrac{\partial(\vec{r}_m)}{\partial(\vec{\rho}_m, \vec{\theta})}$ exist and have rank $3N - 3$.

and the condition that this relation can be solved for $\delta \vec{\theta}$ is that $\tilde{B}$ is non-singular. If the equilibrium configuration was non-linear, then $\tilde{B}(\vec{\rho}_m)$ was non-singular when $\vec{\rho}_m = 0$; and for some neighborhood of the equilibrium, the condition will still apply, and the separation into rotational and vibrational coordinates will be valid.

To complete the transformation into normal coordinates, we transform the velocities

$$\dot{\vec{r}}_m = \frac{d\vec{r}_m}{dt} = \tilde{R}(\theta) \cdot (\frac{d\vec{\theta}}{dt} \times \vec{s}_m + \frac{d\vec{\rho}_m}{dt})$$

and define the angular velocity of the configuration

$$\vec{\omega} = \frac{d\vec{\theta}}{dt}$$

$$\dot{\vec{r}}_m = \tilde{R}(\theta) \cdot (\vec{\omega} \times \vec{s}_m + \dot{\vec{\rho}}_m) ;$$

and since, for any vectors $\vec{a}$ and $\vec{b}$, the scalar product $\vec{a} \cdot \vec{b}$ $= (\tilde{R}(\theta) \cdot \vec{a}) \cdot (\tilde{R}(\theta) \cdot \vec{b})$ is invariant under rotation,

$$T = \frac{1}{2} M(\dot{\vec{X}})^2 + \frac{1}{2} \sum_{m=1}^{N} m_m(\dot{\vec{\rho}}_m^{\,2} + 2 \vec{\omega} \cdot \vec{s}_m \times \dot{\vec{\rho}}_m + (\vec{\omega} \times \vec{s}_m)\cdot(\vec{\omega} \times \vec{s}_m)) .$$

Now define the tensor of inertia

$$\tilde{I} = \sum_{m}^{N} m_m[\tilde{1}(\vec{s}_m \cdot \vec{s}_m) - \vec{s}_m \vec{s}_n] .$$

Then

$$\sum_{m=1}^{n} m_m(\vec{\omega} \times \vec{s}_m) \cdot (\vec{\omega} \times \vec{s}_m) = \vec{\omega} \cdot \tilde{I} \cdot \vec{\omega}$$

and define the 3N - 6 normal coordinates q^i, such that

$$\vec{\rho}_m = \sum_{i=1}^{3N-6} \vec{c}_{mi}\, q^i ,$$

where the $\vec{c}_{mi}$ satisfy:

$$\sum_{m=1}^{N} m_m \vec{c}_{mi} = 0$$

$$\sum_{m=1}^{N} m_m \vec{c}_{mi} \cdot \vec{c}_{mj} = \delta_{ij}$$

$$\sum_{m=1}^{N} m_m \vec{a}_m \times \vec{c}_{mi} = 0$$

$$\sum_{m,n=1}^{N} \vec{c}_{mi} \cdot \tilde{V}_{mn} \cdot \vec{c}_{mj} = V_i \; \delta_{ij} \quad .$$

Note that in the above there are (3N)(3N - 6) components of $\vec{c}_{mi}$ to be determined, together with the 3N - 6 quantities V_i, and that there are exactly (3N + 1)(3N - 6) relations; so that in principle, the separation into normal coordinates can be made.

Lastly, define

$$\vec{\zeta}_{ij} = \sum_{m} m_m \vec{c}_{mi} \times \vec{c}_{mj} \; ; \qquad \zeta_{ij} = - \zeta_{ji} \quad .$$

Then

$$\sum_{m=1}^{N} m_m \vec{\omega} \cdot (\vec{s}_m \times \dot{\vec{\rho}}_m) = \sum_{m=1}^{N} m_m \vec{\omega} \cdot (\vec{\rho}_m \times \dot{\vec{\rho}}_m) = \vec{\omega} \cdot \sum_{i,j=1}^{3N-6} \vec{\zeta}_{ij} \, q_i \dot{q}_j \; ,$$

and

$$T = \frac{1}{2} M(\dot{\vec{X}})^2 + \frac{1}{2} \sum_{ij} \dot{q}^i \delta_{ij} \dot{q}^j + \frac{1}{2} \vec{\omega} \cdot \tilde{I} \cdot \vec{\omega} + \frac{1}{2} \sum_{ij} 2\vec{\omega} \cdot \vec{\zeta}_{ij} \, q^i \dot{q}^j \quad .$$

We omit the center of mass motion from further discussion and define

$$v^{\mu} = \dot{q}^{\mu} \qquad \mu = 1,2, \ldots , 3N - 6$$

$$v^{\mu} = \omega_{x,y,z} \qquad \mu = 3N - 5,\ 3N - 4,\ 3N - 3.$$

We consider i, j = 1, ... , 3N - 6

$$\alpha, \beta = 1,\ 2,\ 3,\ \equiv x,\ y,\ z \; ;$$

and adopt the convention of summation over repeated, lower case, Latin or Greek indices (all equations employing the summation convention are numbered S).

(S) $$T = \frac{1}{2} v^{\mu} T_{\mu\nu} v^{\nu} \qquad T_{\mu\nu} = \begin{pmatrix} 1_{ij} & \zeta^{T}_{i\beta} \\ \zeta_{aj} & I_{a\beta} \end{pmatrix}$$

where

(S) $$\zeta_{aj} = (\vec{\zeta}_{ij}\, q^{i})_{a} \quad .$$

We now define normal momenta p_{μ} , where

$$p_{\mu} = \frac{\partial T}{\partial v^{\mu}} \qquad \mu = 1, \dots , 3N - 3$$

so

(S) $$p_{i} = \frac{\partial T}{\partial \dot{q}^{i}} = \delta_{ij}\, \dot{q}^{i} + \zeta^{T}_{i\beta}\, \omega^{\beta}$$

(S) $$p_{a} = \frac{\partial T}{\partial \omega^{a}} = I_{a\beta}\, \omega^{\beta} + \zeta_{aj}\, \dot{q}^{j} \quad .$$

Then

(S) $$T = \frac{1}{2} p_{\mu}\, T^{\mu\nu}\, p_{\nu} \quad ,$$

where

(S) $$T^{\mu\nu} = (T_{\mu\nu})^{-1} = \begin{pmatrix} \delta^{ij} + \delta^{ik}\, \zeta^{T}_{ia}\, \mu^{a\beta}\, \zeta_{\beta l}\, \delta^{lj} & -\delta^{ik}\, \zeta^{T}_{ka}\, \mu^{a\beta} \\ -\mu^{a\beta}\, \zeta_{\beta l}\, \delta^{lj} & \mu^{a\beta} \end{pmatrix}$$

where

(S) $$\mu^{a\beta} = [I_{a\beta} - \zeta_{aj}\, \delta^{jl}\, \zeta^{T}_{l\beta}]^{-1} = [I - \zeta\zeta^{T}]^{-1}$$

and for later use we note that

$$\mu = ||\mu^{\alpha\beta}|| = ||I - \zeta\zeta^{T}||^{-1} = ||T_{\mu\nu}||^{-1} = ||T^{\mu\nu}|| \quad .$$

Thus

$$(S) \quad T = \frac{1}{2} [p_\alpha \mu^{\alpha\beta} p_\beta - p_i \delta^{ik} \zeta^{T}_{k\alpha} \mu^{\alpha\beta} p_\beta - p_\alpha \mu^{\alpha\beta} \zeta_{\beta l} \delta^{lj} p_j + p_i \delta^{ik} \zeta^{T}_{i\alpha} \mu^{\alpha\beta} \zeta_{\beta l} \delta^{lj} p_j + p_i \delta^{ij} p_j]$$

and if we define

$$(S) \quad \pi_\alpha = p_i \delta^{ik} \zeta^{T}_{i\alpha} = \zeta_{\alpha j} \delta^{jk} p_k = \zeta_{\alpha i j} q^i \delta^{jk} p_k$$

then

$$(S) \quad H = T + V = \frac{1}{2} (p_\alpha - \pi_\alpha) \mu^{\alpha\beta} (p_\beta - \pi_\beta) + \frac{1}{2} p_i \delta^{ij} p_j + \frac{1}{2} \sum_i V_i (q^i)^2 \quad ;$$

p_α is the total angular momentum,

π_α plays the role of an internal angular momentum,

$\mu^{\alpha\beta}$ are related to the inertial tensor but involve the vibrational coordinates in a complex fashion.

2.2. Quantum Mechanical Hamiltonian.

The normal and rotational coordinates of the semi-rigid rotator are not cartesian coordinates and hence demand a special quantization procedure. Although the resulting form of the quantum mechanical Hamiltonian is known, [4] it is often given incorrectly, and a derivation in print is hard to discover. Hence we give the derivation here.

We adopt the viewpoint of tensor calculus, that wherever it is possible in principle to use cartesian coordinates and to obtain generalized coordinates by a suitable coordinate transformation, the resulting Schroedinger's equation, Hamiltonian, and momenta are correct. Any covariant expressions which result from the transformation will then apply to all coordinate systems, even if no cartesian coordinates exist.

2.2.1. Cartesian Coordinates.

Given a set of N particles with

masses m_n $\qquad n = 1, 2, \ldots, N$

we can redefine indices such that the coordinates are denoted by a single index, and are cartesian coordinates in a 3N-dimensional space, i.e., let

$$x^i = x_n^\alpha , \quad \text{where}$$

$$i = \alpha + 3n - 3 , \qquad i = 1, 2, \ldots, 3N.$$

Then in terms of velocities $\dot{x}^i$ and a mass tensor

$$m_{x^i x^j} \equiv \delta_{ij}\, m_{n(i)} \qquad \text{where} \qquad n(i) = \frac{i + 3 - \alpha}{3}$$

$$\text{and} \quad \alpha = 1, 2, 3 ,$$

such that n is an integer

we can express the classical kinetic energy

$$T = \frac{1}{2}\, m_{x^i x^j}\, \dot{x}^i\, \dot{x}^j \tag{S}$$

and momenta

(S) $$p_{x^i} = \frac{\partial T}{\partial \dot{x}^i} = m_{x^i x^j} \delta^j_k \dot{x}^k = m_{n(i)} \dot{x}^i \;;$$

and with the inverse mass tensor

(S) $$m^{x^i x^j} = \delta^{ij} m^{-1}_{(i)} = (m_{x^\cdot x^\cdot})^{-1\, x^i x^j}$$

and the potential

$$V = V(x)$$

we can express the classical Hamiltonian

(S) $$H = T + V = \frac{1}{2} m^{x^i x^j} p_{x^i} p_{x^j} + V(x) \quad .$$

We then form the quantum mechanical momenta and Hamiltonian by writing

$$p_{x^i} = -i\hbar \frac{\partial}{\partial x^i}$$

and introduce a wave function Ψ satisfying Schroedinger's equation

$$H \Psi = E \Psi$$

(S) $$\left(-\frac{1}{2} \hbar^2 m^{x^i x^j} \frac{\partial}{\partial x^i} \frac{\partial}{\partial x^j} + V(x)\right) \Psi_x = E \Psi_x \quad .$$

Wave functions have a scalar product, defined by

$$(\phi_x , \Psi_x) = \int \phi^*_x \Psi_x \, d^{3N} x^i \quad .$$

Any Hermitian operator 0, satisfies

$$(0\phi_x , \Psi_x) = (\phi_x , 0 \Psi_x)$$

For any ϕ and Ψ, and note that p_{x^i} and H as defined are Hermitian.

The momenta in addition, satisfy the commutation relations

$$[p_{x^i} , x^j] = -i\hbar \delta^j_i$$

$$[p_{x^i} , p_{x^j}] = [x^i, x^j] = 0 \quad .$$

2.2.2. General Coordinates.

If now we are given another set of coordinates

$$q^i \qquad i = 1,2, \ldots , 3n$$

in terms of which the classical Hamiltonian is

(S) $$H = \frac{1}{2} \mu^{ij} p_i p_j + V(q)$$

in which $\mu^{ij} = \mu^{ji}$ are functions of q, we can form the quantum mechanical Hamiltonian and momenta by writing the former expressions in covariant form.

First let us introduce the metric tensor

$$g^{ij} \qquad (= \delta^{ij} \text{ in cartesian coordinates})$$

and call

$$g \equiv ||g^{ij}|| \equiv \det g^{ij} \qquad (= 1 \text{ in cartesian coordinates})$$

then, according to the tensor calculus, the volume element transforms to

$$d^{3N} x = g^{-1/2} d^{3N} q$$

and the covariant form for the Schroedinger equation is

(S) $$-\frac{1}{2} \hbar^2 g^{1/2} \frac{\partial}{\partial q^i} m^{ij} g^{-1/2} \frac{\partial}{\partial q^j} \Psi_x + V \Psi_x = E \Psi_x \quad .$$

The above expression, with both m^{ij} and g in it is awkward, but from

(S) $$g^{ij} = \frac{\partial q^i}{\partial x^k} \frac{\partial q^j}{\partial x^l} \delta^{kl}$$

$$(S) \qquad m^{ij} = \frac{\partial q^i}{\partial x^k} \frac{\partial q^j}{\partial x^l} m^{x^i x^l} = \frac{\partial q^i}{\partial x^R} \frac{\partial q^j}{\partial x^l} \delta^{kl} m^{-1}_{n(k)}$$

it follows that

$$m \equiv ||m^{ij}|| = cg \, ,$$

where

$$c = \prod_{n=1}^{N} m_n^3$$

is a constant which commutes with $\frac{\partial}{\partial q^i}$, so that we may write:

$$(S) \qquad H_x \Psi_x = - \frac{\hbar^2}{2} m^{1/2} \frac{\partial}{\partial q^i} m^{ij} m^{-1/2} \frac{\partial}{\partial q^j} \Psi_x + V \Psi_x = E \Psi_x \, .$$

The scalar product of two wave functions must be invariant under coordinate transformation. Hence

$$(\phi_x \, , \Psi_x) = \int \phi_x^* \Psi_x \, g^{-1/2} \, d^{3N} q$$

but if we attempt to identify ϕ_x , Ψ_x as the wave functions and to use its $\partial/\partial q^i$ as momentum operators, we find that although these expressions have the correct commutativity for momenta p_i, they are not Hermitian with respect to wave functions ϕ_x . To resolve the difficulty, we can form new wave functions

$$\bar{\Psi}_q = g^{-1/4} \Psi_x$$

and compute scalar products according to

$$(\bar{\phi}_q \, , \bar{\Psi}_q) = \int \bar{\phi}_q^* \bar{\Psi}_q \, d^{3N} q = (\phi_x \, , \Psi_x) \, .$$

Then the momenta

$$\bar{p}_i = - i\hbar \frac{\partial}{\partial q^i}$$

are Hermitian with respect to wave functions $\bar{\phi}_q$. The appropriate Hamiltonian is then

$$\bar{H}_q = g^{-1/4} H_x g^{1/4} = m^{-1/4} H_x m^{1/4}$$

(S) $$\bar{H}_q = -\frac{\hbar^2}{2} m^{1/4} \frac{\partial}{\partial q^i} m^{ij} m^{-1/2} \frac{\partial}{\partial q^j} m^{1/4} + V$$

(S) $$= \frac{1}{2} m^{1/4} \bar{p}_i m^{ij} m^{-1/2} \bar{p}_j m^{1/4} + V$$

which is Hermitian.

The bars have been used in the above expressions simply because it is not customary to define the scalar product, the momenta and the Hamiltonian in this manner. Instead, one usually regards the wave functions as scalars, and so let

$$\phi_q = \phi_x = g^{1/4} \bar{\phi}_q , \qquad (\phi_q , \Psi_q) = \int \phi_q^* \Psi_q g^{-1/2} d^{3N} q .$$

It then follows that the correct forms for p_i and H_q may be obtained by transforming back from the barred expressions:

$$p_i = g^{1/4} \bar{p}_i g^{-1/4} = -i\hbar m^{1/4} \frac{\partial}{\partial x^i} m^{-1/4}$$

(S) $$H_q = \frac{1}{2} g^{1/4} \bar{H}_q g^{-1/4} = \frac{1}{2} m^{1/4} p_i m^{ij} m^{-1/2} p_j m^{1/4} + V$$

(S) $$= -\frac{\hbar^2}{2} m^{1/2} \frac{\partial}{\partial q^i} m^{ij} m^{-1/2} \frac{\partial}{\partial q^j} + V = H_x .$$

Adopting the more conventional forms, one can drop the subscripts on Ψ and H and so, given the classical Hamiltonian

(S) $$H = \frac{1}{2} m^{ij} p_i p_j + V(q)$$

and the volume element

$$d\tau = g^{-1/2} \, d^{3N} q$$

use

$$p_i = - i\hbar \, m^{1/4} \frac{\partial}{\partial x^i} m^{-1/4}$$

$$\text{(S)} \qquad H = \frac{1}{2} m^{1/4} p_i \, m^{ij} \, m^{-1/2} \, p_j \, m^{1/4} + V(q)$$

$$(\phi, \Psi) = \int \phi^* \, \Psi \, g^{-1/2} \, d^{3N} q \quad .$$

However, if the volume element is unknown, it is possible then to use the unconventional barred forms.

$$\bar{p}_i = - i\hbar^2 \frac{\partial}{\partial q^i}$$

$$\bar{H} = \frac{1}{2} m^{1/4} \bar{p}_i \, m^{ij} \, m^{-1/2} \, \bar{p}_j \, m^{1/4} + V(q)$$

$$(\bar{\phi}, \bar{\Psi}) = \int \bar{\phi}^* \, \bar{\Psi} \, d^{3N} q$$

for which it is necessary to know only the range of the variables q^i .

2.2.3. Momentum Transformation.

For certain systems, the classical Hamiltonian may be written in simpler form if expressed not in terms of a certain set of coordinates and the conjugate momenta, but rather in terms of the coordinates and linear (but coordinate-dependent) combinations of the conjugate momenta.

In particular, this situation occurs in the treatment of the semi-rigid rotator, whose classical Hamiltonian is more simply expressed in terms of cartesian components of angular momentum rather than in angular momenta conjugate to Euler angles.

The new momenta are in general not conjugate to any set of coordinates. (Indeed, quantum mechanically the commutation relations, taken together with the transformation coefficients, form a set of linear partial differential equations which, in general, are non-integrable.) Hence the quantum mechanical Hamiltonian may not be obtained directly from the previous discussion without qualification.

The treatment of this question follows that given by Wilson and Howard, [2] except for the use here of the correct form for the quantum mechanical Hamiltonian.

If we start with the Q.M. Hamiltonian

(S) $$H = \frac{1}{2} m^{1/4} p_i m^{-1/2} m^{ij} p_j m^{1/4} + V$$

and apply the transformation

(S) $$p_i = s_i^m P_m \qquad s_i^m = s_i^m(q)$$

whose inverse is

(S) $$P_m = \gamma_m^i p_i \qquad \gamma_m^i = (s)^{-1}\,{}_m^i \;;$$

define

(S) $$m^{ij} = \gamma_m^i \gamma_n^j M^{mn}$$

where

(S) $$M^{mn} = s_i^m s_j^n m^{ij}$$

and call

$$||\gamma_m^i|| = \gamma \qquad ||s_i^n|| = s = \gamma^{-1} \qquad ||M^{mn}|| = M$$

then

$$m = ||M^{ij}|| = \gamma^2 M$$

therefore

$$2(H - V) = \gamma^{1/2} M^{1/4} s_i^n \acute{P}_n \gamma^{-1} M^{-1/2} \gamma_m^i \gamma_l^j M^{ml} s_j^t \acute{P}_t \gamma^{1/2} M^{1/4}$$

(S) $$= \gamma^{1/2} M^{1/4} s_i^n \acute{P}_n \gamma^{-1} M^{-1/2} \gamma_m^i M^{ml} \acute{P}_l \gamma^{1/2} M^{1/4} .$$

Now if it should turn out that

(S) $$\gamma s_i^k \acute{P}_k \gamma_m^i \gamma^{-1} = \acute{P}_m$$

is true with $\acute{P}_m$'s regarded as differential operators, or

(S) $$\gamma s_i^n \gamma_n^j p_j \gamma_m^i \gamma^{-1} = \gamma_m^k p_k$$

(S) $$\gamma p_j \gamma_m^j \gamma^{-1} = \gamma_m^k p_k$$

(S) $$p_j \gamma_m^j \gamma^{-1} = \gamma_m^k \gamma^{-1} p_k$$

or

$$\sum_J [p_J , \gamma_m^J \gamma^{-1}] = 0 \qquad \text{for all } m ;$$

then

(S) $$2(H - V) = M^{1/4} P_m M^{-1/2} M^{mn} P_n M^{1/4}$$

or

(S) $$H = \frac{1}{2} M^{1/4} P_m M^{-1/2} M^{mn} P_n M^{1/4} + V$$

where

(S) $$P_m = \gamma^{-1/2} \acute{P}_m \gamma^{1/2} = \gamma^{-1/2} \gamma_m^i p_i \gamma^{1/2} .$$

(This is the expected form for the momenta, since if coordinates Q conjugate to P existed we would have had

$$P_m = -i\hbar\, M^{1/4} \frac{\partial}{\partial Q^m}\, M^{-1/4}$$

and

$$M^{1/4} = \gamma^{-1/2}\, m^{1/4}$$

so that the factors $\gamma^{-1/2}$ and $\gamma^{1/2}$ would have entered automatically.)

Lastly, the equation $\sum_J [p_J , \gamma^J_n \; \gamma^{-1}] = 0$ is invariant under simultaneous similarity transformations on p_J and $(\gamma^J_n \gamma^{-1})$ so we may use

$$p_J \to m^{-1/4}\, p_J\, m^{1/4} = -i\hbar \frac{\partial}{\partial q^J}$$

$$\gamma^J_n \; \gamma^{-1} \to \gamma^J_n \; \gamma^{-1}$$

and write

$$\sum_J \frac{\partial}{\partial q^J} (\gamma^J_n \; \gamma^{-1}) = 0 \quad \text{as the required condition.}$$

To summarize, we may say that if a classical momentum transformation

$$P_m = \gamma^i_m\, p_i \qquad\qquad s^i_m = (\gamma^{\cdot}_{\cdot})^{-1}{}^{i}_{m} \qquad\qquad \gamma = || \gamma^{\cdot}_{\cdot} ||$$

satisfies

(S) $$\frac{\partial}{\partial q^i} (\gamma^i_j \; \gamma^{-1}) = 0 \quad \text{for all } j$$

and if we denote

(S) $$M^{mn} = s^m_i\, s^n_j\, m^{ij} \qquad\qquad M = \gamma^{-2}\, m$$

then if in terms of the old variables

(S) $$H = \frac{1}{2}\, m^{1/4}\, p_i\, m^{ij}\, m^{-1/2}\, p_j\, m^{1/4} + V(q)$$

we may use

(S) $$H = \frac{1}{2} M^{1/4} P_m M^{mn} M^{-1/2} P_n M^{1/4} + V(q)$$

where

(S) $$P_m = \gamma^{-1/2} \gamma^i_m p_i \gamma^{1/2} ,$$

and use the old wave functions and inner products

$$(\emptyset, \Psi) = \int \emptyset^* \Psi \, d\tau \ (q).$$

Alternatively, we may employ the Hamiltonian and momentum operators given by

(S) $$H' = \frac{1}{2} M^{1/4} P'_m M^{mn} M^{-1/2} P'_n M^{1/4} + V(q)$$

(S) $$P'_m = \gamma^i_m p_i ;$$

provided that we transform the wave functions according to

$$\Psi' = \gamma^{1/2} \Psi$$

and use the inner product

$$(\Psi', \emptyset') = \int \Psi'^* \emptyset' \gamma^{-1} d\tau \, (q).$$

In the treatment of the semi-rigid rotator, the natural coordinates are the normal coordinates of vibration q^i and the Euler angles $(\emptyset, \theta, \Psi)$. The Hamiltonian is more easily expressed in terms of cartesian angular momenta in a system of coordinates rotating with the configuration, $P_{x'}$, $P_{y'}$, $P_{z'}$, for which the classical transformation is:

$$P_{x'} = \sin \Psi \, p_\theta - \cos \Psi \csc \theta \, p_\emptyset + \cos \Psi \cot \theta \, p_\Psi$$
$$P_{y'} = \cos \Psi \, p_\theta + \sin \Psi \csc \theta \, p_\emptyset - \sin \Psi \cot \theta \, p_\Psi$$
$$P_{z'} = p_\Psi$$

or, taking 1, 2, 3 ≡ ϕ, θ, Ψ

$$P_\alpha = \gamma^\beta_\alpha \, p_\beta \quad , \qquad \text{where}$$

$$\gamma^\beta_\alpha = \begin{pmatrix} \sin\Psi & -\cos\Psi \csc\theta & \cos\Psi \cot\theta \\ \cos\Psi & \sin\Psi \csc\theta & -\sin\Psi \cot\theta \\ 0 & 0 & 1 \end{pmatrix}$$

$$\gamma = \csc\theta \quad .$$

Computing

$$\frac{\partial}{\partial q^\beta} (\gamma^\beta_\alpha \; \gamma^{-1}) \; ,$$

we get

$$\frac{\partial}{\partial\theta} \sin\Psi \sin\theta + \frac{\partial}{\partial\phi} (-\cos\Psi) + \frac{\partial}{\partial\Psi} (\cos\Psi \cos\theta) = 0$$

$$\frac{\partial}{\partial\theta} \cos\Psi \cos\theta + \frac{\partial}{\partial\phi} (\sin\Psi) + \frac{\partial}{\partial\Psi} (-\sin\Psi \cos\theta) = 0$$

$$\frac{\partial}{\partial\Psi} (\sin\theta) = 0 \quad ;$$

verifying that this is one of the allowed momentum transformations.

The metric determinant of the Euler coordinates is

$$g = R \sin^2\theta$$

where R is not a function of θ, ϕ, Ψ although it may involve configurational coordinates. Thus the quantum mechanical Euler momenta are

$$p_{\theta,\phi,\Psi} = - i\hbar \, (\sin\theta)^{-1/2} \; \frac{\partial}{\partial\theta, \, \phi, \, \Psi} \; (\sin\theta)^{1/2}$$

but since $\gamma = (\sin\theta)^{-1}$, we form the quantum mechanical cartesian angular momenta by

$$P_\alpha = \gamma^{-1/2}\ \gamma_\alpha^\beta\, p_\beta\ \gamma^{1/2} = (\sin\theta)^{1/2}\, \gamma_\alpha^\beta\, p_\beta\, (\sin\theta)^{-1/2}$$

$$= -i\hbar\, \gamma_\alpha^\beta \frac{\partial}{\partial\theta^\beta} \qquad \alpha = x', y', z'$$

$$= -i\hbar \frac{\partial}{\partial\theta'_\alpha} \qquad \beta = \theta, \phi, \Psi$$

which are simple derivative operators with respect to infinitesimal rotations about the x', y', z' axes.

3.0. The Complete Quantum Mechanical Hamiltonian.

As a result of the above considerations, we can write the quantum mechanical Hamiltonian as

$$H = \frac{1}{2} \sum_{\alpha,\beta=1}^{3} \mu^{1/4}(p_\alpha - \pi_\alpha)\,\mu^{-1/2}\,\mu^{\alpha\beta}\,(p_\beta - \pi_\beta)\,\mu^{1/4}$$

$$+ \frac{1}{2} \sum_{i,j=1}^{3N-6} \mu^{1/4}\, p_i\, \mu^{-1/2}\, p_i\, \mu^{1/4} + \frac{1}{2} \sum_{i=1}^{3N-6} V_i^{(o)} (q^i)^2$$

$$+ \sum_{i,j,k=1}^{3N-6} V_{ijk}^{(1)}\, q^i\, q^j\, q^k + \sum_{i,j,k,l=1}^{3N-6} V_{ijkl}^{(2)}\, q^i\, q^j\, q^k\, q^l + \cdots$$

where q^i, $i = 1, \ldots, 3N-6$ are the internal coordinates

$\mu^{\alpha\beta}$ is the inertial tensor

$\mu = ||\mu^{\alpha\beta}||$

$p_i = -i\hbar\, \mu^{-1/4} \frac{\partial}{\partial q^i}\, \mu^{1/4}$ are the momenta

$p_\alpha = -i\hbar \frac{\partial}{\partial\theta'_\alpha}$ are operators for total angular momentum components about the body axes.

$$\pi_\alpha = \sum_{i,j=1}^{3N-6} \zeta_{\alpha ij}\, q^i\, p_j\,, \quad \text{or} \quad \vec{\pi} = \sum_{i,j=1}^{3N-6} \vec{\zeta}_{ij}\, q^i\, p_j$$

represent components of internal angular momentum about the body axes.*

$V_i^{(o)}$ are potential coefficients of lowest order.

$V_{ijk}^{(1)}$, $V_{ijkl}^{(2)}$ are coefficients of higher order expansion of the potential function.

3.1. Perturbation Expansion.

Since the complete Schroedinger equation cannot be solved exactly, it is necessary to perform a perturbation expansion in q_i in which it is assumed that the most important terms are those which arise from the coordinate-independent part of $\mu^{\alpha\beta}$ and the quadratic terms in the potential expansion, and that other terms, which involve higher powers of q^i, produce smaller effects.

First note, that for any $\mu^{\alpha\beta} = \mu^{\beta\alpha}(q)$, and $\pi_\alpha = \pi_\alpha(p, q)$ linear in p:

$$\sum_{\alpha\beta} \mu^{1/4}\, \pi^\alpha \mu^{\alpha\beta} \mu^{-1/2}\, \pi^\beta \mu^{1/4} = \sum_{\alpha\beta} \Big\{ \mu^{\alpha\beta}\, \pi^\alpha\, \pi^\beta$$

$$- \frac{5}{16}\, \mu^{\alpha\beta}\, \mu^{-2} [\pi_\alpha , \mu\,][\pi_\beta , \mu] + \frac{1}{4}\, \mu^{\alpha\beta}\, \mu^{-1} [\pi_\alpha\,, [\pi_\beta\,, \mu\,]]$$

$$+ [\pi_\alpha\,, \mu^{\alpha\beta}\,]\, \pi^\beta + \frac{1}{4}\, \mu^{-1}\, [\pi_\alpha\,, \mu^{\,\alpha\beta}]\, [\pi_\beta\,, \mu] \Big\} \quad .$$

---

* However, see condition (2), Sect. I, 3.2.

Thus also

$$\sum_i \mu^{1/4} p^i \mu^{-1/2} p^i \mu^{1/4} = \sum_i \left\{ p_i^2 - \frac{5}{16} \mu^{-2} [p_i , \mu]^2 + \frac{1}{4} \mu^{-1} [p_i , [p_i , \mu]] \right\} .$$

Lastly, since $[p_\alpha , \mu^{\alpha\beta}] = [p_\alpha , \mu] = [p_\alpha , \pi_\beta] = 0$

$$\sum_{\alpha\beta} \mu^{1/4} (p_\alpha \mu^{-1/2} \mu^{\alpha\beta} \pi_\beta + \pi_\alpha \mu^{-1/2} \mu^{\alpha\beta} p_\beta) \quad ^{1/4}$$

$$= \sum_{\alpha\beta} \left\{ \mu^{\alpha\beta} p_\alpha \pi_\beta + [\pi_\alpha , \mu^{\alpha\beta}] p_\beta - \frac{1}{4} \mu^{\alpha\beta} \mu^{-1} [\pi_\alpha , \mu] p_\beta \right\} .$$

All terms which involve $[p_\alpha, \mu]$, $[\pi_\alpha , \mu]$ etc. are to be treated as higher order terms; thus let

$$\mu^{\alpha\beta} = \mu_o^\alpha \, \delta^{\alpha\beta} + \mu_1^{\alpha\beta} + \mu_2^{\alpha\beta} + \cdots$$

$$\mu = \mu_o (1 + \mu_1 + \mu_2 + \cdots)$$

where since no generality is lost by doing so, we take $\mu_o^{\alpha\beta}$ as diagonal, and where μ_1, $\mu_1^{\alpha\beta}$ involve q^i in first order; μ_2, $\mu_2^{\alpha\beta}$ in second order, etc.; and perform a second order expansion.

Then

$$H = H_o' + H_1' + H_2' , \qquad \text{where}$$

$$2H_o' = \sum_{\alpha=1}^{3} \mu_o^\alpha (p_\alpha - \pi_\alpha)(p_\alpha - \pi_\alpha) + \sum_i (p_i^2 + V_i^{(o)} q_i^2)$$

$$2H_1' = \sum_{\alpha,\beta=1}^{3} \left\{ \mu_1^{\alpha\beta} (p_\alpha - \pi_\alpha)(p_\beta - \pi_\beta) - [\pi_\alpha, \mu_1^{\alpha\beta}] (p_\beta - \pi_\beta) - \frac{1}{4} \mu_o^\alpha [\pi_\alpha , \mu_1] \, \delta^{\alpha\beta} \, p_\beta \right\} + \sum_{ijk} V_{ijk} q_i q_j q_k$$

$$
\begin{aligned}
2H_2' = \sum_{\alpha,\beta=1}^{3} \Big\{ & -\frac{5}{16}\mu_o^{\alpha}\, \delta^{\alpha\beta}\, [\pi_\alpha , \mu_1]^2 + \frac{1}{4}\mu_o^{\alpha}\, \delta^{\alpha\beta} [\pi_\alpha , [\pi_\alpha , \mu_2]] \\
& + \frac{1}{4}[\pi_\alpha , \mu_1^{\alpha\beta}][\pi_\beta , \mu_1] + \mu_2^{\alpha\beta}\, (p_\alpha - \pi_\alpha)(p_\beta - \pi_\beta) \\
& - [\pi_\alpha , \mu_2^{\alpha\beta}](p_\beta - \pi_\beta) - \frac{1}{4}\mu_1^{\alpha\beta}[\pi_\alpha , \mu_1]p_\beta - \frac{1}{4}\mu_o^{\alpha}\delta^{\alpha\beta}[\pi_\alpha , \mu_2]p_\alpha \\
& + \sum_{i=1}^{3N-6} \Big\{ -\frac{5}{16}[p_i , \mu_1]^2 + \frac{1}{4}[p_i , [p_i , \mu_2]] \Big\} \\
& + \sum_{i,j,k,l=1}^{3N-6} V_{ijkl}\, q^i q^j q^k q^l \quad .
\end{aligned}
$$

Lastly, one must take into account the existence of degeneracy: the Hamiltonian in terms of which the perturbation expansion is made is

$$H_o^o = \frac{1}{2} \sum_{\alpha} p_\alpha \mu_o^{\alpha} p_\alpha + \frac{1}{2} \sum_{i} (p_i^2 + V_i^{(o)} q_i^2)$$

and if some of the V_i's are equal, those perturbation terms which involve only a single degenerate group will have to be treated differently from others.

Thus we further define

$$\pi_\alpha = \pi_\alpha^o + \pi_\alpha^1$$

where π_α^o mixes only states within the same degenerate group, while π_α^1 mixes states belonging to different groups. And then we redefine

$$H_o = \frac{1}{2} \sum_{\alpha=1}^{3} \mu_o^{\alpha}(p_\alpha - \pi_\alpha^o)(p_\alpha - \pi_\alpha^o) + \frac{1}{2} \sum_{i} (p_i^2 + V_i^{(o)} q_i^2)$$

$$H_1 = H_1' + \sum_{\alpha=1}^{3} \mu_o^{\alpha}(p_\alpha - \pi_\alpha^1)$$

$$H_2 = H_2' + \frac{1}{2} \sum_{\alpha=1}^{3} \mu_o^{\alpha}\, \pi_\alpha^1\, \pi_\alpha^1$$

In any particular problem, H_o is used as the zeroth order Hamiltonian, but which of the terms in H_1 and H_2 are of significance depends on the particular parameters involved. (For example, it might turn out that one of the terms of H_2 mixed only states of the same degeneracy group.)

3.2. The Zeroth Order Hamiltonian, Further Considerations.

The eigenfunctions of

$$H_o^o = \frac{1}{2} \sum_{\alpha} p_\alpha \mu_o^\alpha p_\alpha + \frac{1}{2} \sum_{i=1}^{3N-6} (p_i^2 + V_i^{(o)} q_i^2)$$

are well known to be

$$\Psi^{Jmk}_{n_1, n_2, \ldots, n_{3N-6}} = \prod_{i=1}^{3N-6} \Psi_{in_i}(q_i) \quad \chi^{Jmk}(\Gamma)$$

where Ψ_{in_i} is the n_i-th harmonic oscillator wave function

$\chi^{Jmk}(\Gamma)$ is an asymmetric top wave function of total angular momentum J, z-component m, index k,

or if, $\mu_o^1 = \mu_o^2$, then $\chi^{Jmk}(\Gamma)$ becomes the symmetric top wave function $Y_J^{mk}(\Gamma)$, also called generalized Legendre function, and k becomes the component of angular momentum about the figure axis.

For the complete zeroth order Hamiltonian

$$H_o = H_o^o + \frac{1}{2} {}_{\alpha=1}^{3} \quad {}_{o}^{\alpha} \pi_\alpha^{o2} + {}_{\alpha=1}^{3} \quad {}_{o}^{\alpha} p_\alpha \pi_\alpha^{o} ,$$

the solution is simple if:

1. $\mu_o^1 = \mu_o^2$ so that $Y_J^{mk}(\Gamma)$ belongs to a definite angular momentum component about the symmetry axis, and,

2. $[\pi_\alpha , \pi_\beta] = \varepsilon_{\alpha\beta\gamma} \sum_{ij} k_{ij} \zeta_{\gamma ij} q^i p_j$, where k_{ij} is independent of γ, q.* In this case,

$$\pi^{o^2}, \quad \sum_{\alpha=1}^{3} \mu_o^\alpha \pi_\alpha^2 , \quad \sum_{\alpha=1}^{3} \mu_o^\alpha p_\alpha \pi_\alpha^o$$

are all simultaneously diagonizable, and $[\pi^{o^2} , \pi_\alpha^o] = 0$, so that the eigenfunctions may be found by the usual methods for combining angular momentum.

The first condition in general, does not apply, but there are many interesting problems in which it does. The second **condition** is probably true in general. The author has been unable to find reference to it in the literature, and neither to prove it in general, nor to discover a counter-example.

Note that even where the second condition applies it is not in general, true that the coordinates q^i of a given degenerate group combine in any familiar fashion, but commonly, a set of three will be found that combine in the same manner as cartesian coordinates.

4.0. Identical Particles. Symmetry Properties and Allowed States.

If the particles are identical, then it is required that the total wave function for vibration plus rotation be symmetric or anti-symmetric in any interchange of the coordinates of the particles

---

* By applying the commutation rules for p_i , q_i to the expression for $[\pi_\alpha , \pi_\beta]$, we find that this condition can be written more simply as:

$$\sum_{j=1}^{3N-6} (\vec{\zeta}_{ij} \times \vec{\zeta}_{kj}) \times \vec{\zeta}_{ik} = 0 \text{ for all i, k.}$$

This algebraic identity is verified in the particular problem considered below.

according as the particles obey Bose or Fermi Statistics, respectively. We treat only the Bose case here since it directly applies to the problem at hand, and since the Fermi case would be slightly more complicated in requiring the introduction of spin coordinates.

The requirement of Bose symmetry severely restricts the number of possible states of the system. The use of group theory will facilitate determination of possible states, and, together with explicit expressions for the vibrational and rotational wave functions, will readily allow us to exhibit the total wave functions for use in later calculations.

4.1. Group Theoretical Method.

The permutations S of the N particles form a group P which is isomorphic with the abstract group P_N of permutations of N things. Since the particles are identical, the vibrational Hamiltonian H_V, the rotational Hamiltonian H_R, the vibration-rotation interaction Hamiltonian H_{RV}, and the total Hamiltonian are invariant under P. We require that out of products of vibrational wave functions $\Psi(q)$ which are eigenfunctions of H_V and rotational wave functions $\Psi(\Theta)$ which are eigenfunctions of H_R are formed those combinations which are invariant under P, and which are also eigenfunctions of H_{RV}.

In general there can be found in P a subgroup R composed of those permutations which correspond to rotations or rotations plus inversions and which form therefore a subgroup R of the complete rotation group. If the rotational coordinates have been properly chosen, there can also be found in P a subgroup C of permutations under which the rotational coordinates (schematically indicated here by θ) are invariant, so that C represents a change in internal configuration with no accompanying rotation. The subgroups R and C will then span the group P, i.e., for any S of P, there is a unique factorization:

$$S = S_R\, S_C = S'_C\, S'_R$$

in which

$S_R(S'_R)$ is an element of R,

$S_C(S'_C)$ is an element of C.

Since $\Psi(\theta)$ is invariant under C, it follows that $\Psi(q)$ must be invariant under C as well, but only the product wave function must be invariant under R and hence under the full group P.

In the particular problems of O^{16} on the α-particle model it turns out that R is identical with P. Hence we shall use S to indicate a group element, and P to indicate the group, although in the general case we should have to use S_C and R. Also, although in general, we should have to pre-symmetrize $\Psi(q)$ over C, no such procedure is necessary here.

4.1.1. Vibrational Wave Functions.

Since the vibrational Hamiltonian H_V is invariant under P, the vibrational wave functions $\Psi(q)$ must transform under a permutation S by means of the unitary transformation U(S):

$$S\,\Psi = \Psi(Sq) = U(S)\,\Psi(q)$$

which mixes only states belonging to the same energy level E of H_V.

Hence we need confine the discussion only to states $\Psi_E(q)$ of a single degenerate vibrational group.

Further there must exist a unitary transformation V:

$$\Psi_E' = V \, \Psi_E$$

$$U'(S) = V \, U(S) \, V^{-1}$$

which reduces U(S) to block form U'(S) such that each block of U'(S) belongs to an irreducible representation U_α of P. Each irreducible representation will, in general, appear $n^E(\alpha)$ times ($n^E(\alpha)$ is zero or a positive integer):

$$U'(S) = \sum_\alpha \sum_{k'=o}^{n^E(\alpha)} \delta_{kk'} \, U_\alpha(S)$$

$$\Psi_E'(q) = \sum_\alpha \sum_{k=1}^{n^E(\alpha)} \Psi_{E\alpha k}(q)$$

in which $\Psi_{E\alpha k}$ is a vector of orthonormal wave functions transforming under P according to

$$S \, \Psi_{E\alpha k}(q) = \Psi_{E\alpha k}(Sq) = U_\alpha(S) \, \Psi_{E\alpha k}(q) \quad .$$

4.1.2. Rotational Wave Functions.

We shall confine our discussion to the spherical top case in which the three moments of inertia are equal. In addition to being the one immediately applicable to O^{16}, it is the most interesting mathematically because the greatest degree of rotational degeneracy occurs.

In the spherical top, the rotational energy depends solely upon the total angular momentum J. The rotational wave functions Ψ_J^{km},

m fixed, $|m| \leq J$, $k = -J, -J+1, \dots , J-1, J$ transform according to the irreducible representation D_J of the rotation group. Under the subgroup P (in general R), D_J is reducible, i.e., there exists a unitary matrix V (which connects states of the same m and J values but different k values) which brings $D_J(S)$ into block form such that each block belongs to an irreducible representation U of P. As before:

$$D'_J(S) = V\, D_J(S)\, V^{-1} = \sum_{\beta} \sum_{j=o}^{n^J(\beta)} \delta_{ij}\, U_{\beta}(S)$$

$$\Psi'^{m}_{J}(\theta) = V\, \Psi^{m}_{J}(\theta) = \sum_{\beta, j} \Psi^{m}_{J\beta j}(\theta)$$

$$S\, \Psi^{m}_{J\beta j} = \Psi^{m}_{J\beta j}(S\theta) = U\ (S)\ \Psi^{m}_{J\beta j}(\theta)$$

and the matrices $U_\beta(S)$ are to be chosen identical with the $U_\alpha(S)$ for $\beta = \alpha$.

4.1.3. Total Wave Function.

A stationary state wave function must belong to a particular E value and a particular J value. Further it must be invariant under P. The following conditions can occur:

1. $n^E(\alpha)\, n^J(\alpha) = 0$ for all α. There is no common irreducible representation. A state E, J is then forbidden by the symmetry requirement, since no invariant can be formed.

2. $n^E(\beta)\, n^J(\beta) = \delta_{\alpha\beta}$. For any m value, there is a unique symmetric wave function* which is automatically also an eigenfunction of the rotation-vibration interaction Hamiltonian H_{RV}.

$$\Psi^m_{EJ}(\theta, q) = \tilde{\Psi}_{E\alpha}(q)\, \Psi^m_{J\alpha}(\theta)$$ ~ denotes Hermitian adjoint.

$$S\, \Psi^m_{EJ} = \Psi^m_{EJ}(S\theta, Sq) = \tilde{\Psi}_{E\alpha}(q)\, U^{-1}_{\alpha}(S)\, U_{\alpha}(S)\, \Psi^m_{J_\alpha}(\theta) = \Psi^m_{EJ}(\theta, q).$$

3. $n^E(\beta)\, n^J(\beta) = \sum_{i=1}^{n} \delta_{\beta \alpha_i}$ n symmetric states exist, of the form

$$\Psi^m_{EJ\alpha_i} = \tilde{\Psi}_{E\alpha_i}\, \Psi^m_{J\alpha}.$$

Degeneracy between these states may be removed by the rotation-vibration interaction.

4. $n^E(\alpha)\, n^J(\alpha) > 1$. There is a further degeneracy of order $n^E(\alpha)\, n^J(\alpha)$. Possible states are:

$$\Psi^m_{EJij} = \tilde{\Psi}_{E\alpha k}\, \Psi^m_{J\alpha k'} \qquad \begin{array}{l} k = 1, \ldots, n^E(\alpha) \\ k' = 1, \ldots, n^J(\alpha). \end{array}$$

Degeneracy between these cannot be removed by the vibration-rotation interaction.

---

[*] The proof of the assertion follows directly from Schur's Lemma: Let the wave function be $\Psi = (\Psi_{J\alpha})\, W(\Psi_{E\beta})$. If Ψ is invariant under P, then we have

$$U^{-1}_{\alpha}(S)\, W\, U_{\beta}(S) = W \quad \text{for all } S \text{ in } P,$$

or

$$W\, U_{\beta}(S) = U_{\alpha}(S)\, W \quad \text{for all } S \text{ in } P.$$

(1) If $\alpha \neq \beta$, U_α and U_β are by definition inequivalent irreducible representations of P. By Schur's Lemma, W = 0.

(2) If $\alpha = \beta$ then by Schur's Lemma, W is a multiple of the unit matrix. Since $\Psi_{J\alpha}$ and $\Psi_{E\alpha}$ are orthonormal separately and if Ψ is normalized also, then it is required that W is unitary. Hence W = 1.

To apply these results, we need to determine the numbers $n^E(\alpha)$ and $n^J(\alpha)$ and the wave functions $\Psi_{E\alpha k}$ and $\Psi^m_{J\alpha k}$, which belong to the α-irreducible representations.

Let

R denote an arbitrary unitary representation of a group P.

α denote a particular irreducible unitary representation of P.

h = the order of the group.

$\chi_R(S)$ = the character of S in the R representation

$\chi_\alpha(S)$ = the character of S in the α representation called a primitive character.

Then the number of times the α irreducible representation is included in the α representation is given by

$$n^R(\alpha) = \frac{1}{h} \sum_S \chi^*_\alpha(S) \; \chi_R(S)$$

* denotes the complex conjugate

or if we make use of the fact that χ's are dependent only on the class of group elements and

h(S) = number of elements in class of S

$$n^R(\alpha) = \frac{1}{h} \sum_{\text{classes}} h(S) \; \chi^*_\alpha(S) \; \chi_R(S) \; .$$

4.2. Method of Finding Wave Functions.

In addition to determining $n^R(\alpha)$ we can determine explicitly the basis functions Ψ^R_α of the α representation (or $\Psi^R_{\alpha k}$, $k = 1, \ldots, n(\alpha)$ if $n(\alpha) > 1$).

Given any set of basis functions for the R representation

$$\Psi^R_i, \qquad i = 1, 2, \ldots, N;$$

the decomposition property allows us to write

$$\Psi_i^R = \sum_{\alpha} \sum_{k=1}^{n(\alpha)} \sum_{l=1}^{g(\alpha)} V_{ilk}^{\alpha} \, \Psi_{\alpha kl}^{R} \text{ , where}$$

$g(\alpha)$ = order of the α representation, and

$$\sum_{\alpha} g(\alpha) \, n(\alpha) = N \; .$$

Then

$$S \, \Psi_i^R = \sum_{\alpha} \sum_{k=1}^{n(\alpha)} \sum_{l,l'=1}^{g(\alpha)} V_{ikl}^{\alpha} \, U_{ll'}^{\alpha}(S) \, \Psi_{\alpha kl'}^{R} \; .$$

Now form

$$(\Psi_i^R)_{\beta} = \frac{g(\beta)}{h} \sum_{S} \chi^{*}(S) \, S \, \Psi_i^R = \frac{g(\beta)}{h} \sum_{S} \sum_{\alpha} \sum_{k=1}^{n(\alpha)} \sum_{l,l'=1}^{g(\alpha)} V_{ikl}^{\alpha} \; \chi_{\beta}^{*}(S) \, U_{ll'}^{\alpha}(S) \, \Psi_{\alpha kl'}^{R}$$

Burnside's theorem states:

$$\frac{1}{h} \sum_{S} U_{LL'}^{*}(S) \, U_{ll'}^{\alpha}(S) = \frac{1}{g(\beta)} \, \delta_{\alpha\beta} \; \delta_{Ll} \; \delta_{L'l'}$$

hence

$$\frac{g(\beta)}{h} \sum_{S} U_{LL}^{*}(S) \, U_{ll'}^{\alpha}(S) = \delta_{\alpha\beta} \; \delta_{Ll} \; \delta_{ll'} \quad ,$$

and upon summation over L we get

$$\frac{g(\beta)}{h} \sum_{S} \chi_{\beta}^{*}(S) \, U_{ll'}^{\alpha}(S) = \delta_{\alpha\beta} \; \delta_{ll'} \quad .$$

Applying this result to the S-summation for $(\Psi_i^R)_{\beta}$, we get

$$(\Psi_i^R)_{\beta} = \sum_{k=1}^{n(\beta)} \sum_{l=1}^{g(\beta)} V_{ikl}^{\beta} \, \Psi_{kl}^{R} \qquad i = 1, \ldots , N \; .$$

Thus $(\Psi_i^R)_\beta$ is in fact the projection of (Ψ_i^R) onto the irreducible representation β .

Now to determine a suitable set of functions $\Psi_{\alpha kl}^R$, we first compute $(\Psi_i^R)_\alpha$, $i = 1,2, \ldots , N$; note that there must be exactly $n(\alpha)\, g(\alpha)$ linearly independent functions among them. (There can be no more than this number since they are linear combinations of Ψ_{kl}^R ; there can be no fewer, since the N original Ψ_i^R are all linearly independent, $\sum_\alpha n(\alpha)\, g(\alpha) = N$, and $\sum_\alpha (\Psi_i^R)_\alpha = \Psi_i^R$.) There are two cases to consider:

1. <u>$n(\alpha) = 1$</u> .

If $n(\alpha) = 1$ there are exactly $g(\alpha)$ linearly independent functions among the $(\Psi_i^R)_\alpha$. Any orthonormalized set of $g(\alpha)$ of the $(\Psi_i^R)_\alpha$ can form the bases $\Psi_{\alpha l}^R$, $l=1, \ldots , g(\alpha)$ of the α representation.

2. <u>$n(\alpha) > 1$</u> .

If $n^R(\alpha) > 1$, then there are $n^R(\alpha)\, g(\alpha)$ linearly independent $(\Psi_i^R)_\alpha$. An orthonormalized set of $n^R(\alpha)\, g(\alpha)$ of these functions can be chosen as before, but a further linear transformation on the set is required to reduce the transformations under S to block form.

Call $\phi_{\alpha j}^R$, $j = 1, \ldots , n(\alpha)\, g(\alpha)$ a set of orthonormalized $(\Psi_i^R)_\alpha$ and then let them transform under the group P by

$$S\, \phi_{\alpha j}^R = \sum_{j=1}^{n(\alpha)\, g(\alpha)} \bar{U}_{jj'}^{\alpha}(S)\, \phi_{\alpha j'}^R \quad .$$

We wish to determine a unitary matrix

$$V^{\alpha}_{jkl} , \quad j = 1, \dots , n(\alpha)\, g(\alpha);\ k = 1, \dots , n(\alpha);$$
$$l = 1, \dots , g(\alpha)$$

(k and l together span the space of j, so the unitarity expresses itself as:

$$\sum_{kl} V^{*\alpha}_{jkl}\, V^{\alpha}_{j'kl} = \delta_{jj'}$$
$$\sum_{j} V^{*\alpha}_{jkl}\, V^{\alpha}_{jk'l} = \delta_{kk'}\, \delta_{ll'}),$$

and basis functions

$$\Psi^{R}_{\alpha kl} = \sum_{j=1}^{n(\alpha)\, g(\alpha)} V^{*\alpha}_{jkl}\, \phi^{R}_{\alpha j}$$

and for the particular reduced representation

$$S(\Psi^{R}_{\alpha kl}) = \sum_{l'=1}^{g(\alpha)} U^{\alpha}_{ll'}(S)\, \Psi^{R}_{\alpha kl'} , \qquad k = 1, \dots , n(\alpha) .$$

We then have

$$\bar{U}^{\alpha}_{jj'}(S) = \sum_{k,k'=1}^{n(\alpha)} \ \sum_{l,l'=1}^{g(\alpha)} V^{\alpha}_{jkl}\, U^{\alpha}_{ll'}\, \delta_{kk'}\, V^{*\alpha}_{jk'l} ,$$

and the V's can be determined by applying Burnside's Theorem:

$$\frac{g(\alpha)}{h} \sum_{S} U^{*\alpha}_{LL'}(S)\, \bar{U}^{\alpha}_{jj'}(S) = \sum_{k=1}^{n(\alpha)} V^{\alpha}_{jkL}\, V^{*\alpha}_{j'kl'} .$$

The quantities on the left are presumably known, and the equations determine the V^{α}_{jkl} to within an arbitrary $n(\alpha) \times n(\alpha)$ unitary matrix, i.e., if V_{ikl} is a solution and $W_{kk'}$ is an arbitrary unitary matrix, then $\sum_{k=1}^{n(\alpha)} V_{jk'l}\, W_{k'k}$ is also a solution, a situation resulting from the $n(\alpha)$ fold degeneracy.

PART II. O^{16} ENERGY LEVELS.

1. Application and Computations for O^{16}.

The procedure we shall follow in computing the energy levels and transition rates for O^{16} involves the following steps:

(1) Determination of classical normal modes.

(2) Expression of quantum mechanical wave functions.

(3) Symmetrization; use of group properties of vibration and rotation wave functions to find the eigenvalues of the Hamiltonian.

(4) Explicit representation of the permutation group; formation of wave functions.

(5) Expression of operators for electromagnetic radiation and pair emission in terms of the normal coordinates and rotation operators.

(6) Calculation of lifetimes.

Since we shall need to make use of the properties of and explicit expressions for the generalized Legendre functions (symmetric top wave functions) a derivation of them following a paper by Takehashi [5] is given in Appendix I.

2.0. Classical Normal Modes.

Here we are interested in the configuration of four α-particles which in equilibrium are arranged in a regular tetrahedron. Let

$\vec{x}_n$, $n = 1, \ldots , 4$ be the coordinates of the particles.

To eliminate motion of the C.M. and at the same time produce independent coordinates, let

$$\begin{pmatrix} \vec{\rho}_1 \\ \vec{\rho}_2 \\ \vec{\rho}_3 \\ \vec{R} \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \vec{x}_1 \\ \vec{x}_2 \\ \vec{x}_3 \\ \vec{x}_4 \end{pmatrix}$$

so that $\vec{x}_n = \vec{r}_n + \vec{R}$, where

$\vec{R}$ is the position of the C.M., which will be neglected hereafter, and

$$\begin{pmatrix} \vec{r}_1 \\ \vec{r}_2 \\ \vec{r}_3 \\ \vec{r}_4 \end{pmatrix} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \vec{\rho}_1 \\ \vec{\rho}_2 \\ \vec{\rho}_3 \end{pmatrix} \quad ;$$

are the coordinates of the particles with respect to the C.M. and the combinations $\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3,$ are independent.

Note that $\sum_{n=1}^{4} \vec{r}_n \, \vec{r}_n = 4 \sum_{\alpha=1}^{3} \vec{\rho}_\alpha \, \vec{\rho}_\alpha$ (outer products).

2.1. Kinetic and Potential Energies.

The kinetic energy is given by:

$$T = \frac{1}{2} 4M \sum_{\alpha=1}^{3} \dot{\vec{\rho}}_\alpha \cdot \dot{\vec{\rho}}_\alpha \quad .$$

In order to express the potential energy, we must first consider the equilibrium configuration.

Let a = radius of equilibrium configuration and let

$$\begin{pmatrix} \vec{\rho}_{1o} \\ \vec{\rho}_{2o} \\ \vec{\rho}_{3o} \end{pmatrix} = a \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix} ,$$

where

o subscript refers to equilibrium, and

$\hat{i}', \hat{j}', \hat{k}'$ are a right-handed set of orthogonal unit vectors.

Define

$l_o = 2 \sqrt{\frac{2}{3}}\ a$ = length of side of equilibrium tetrahedron

$$l_1 = |\vec{r}_4 - \vec{r}_1| - l_o = 2|\vec{\rho}_2 + \vec{\rho}_3| - l_o$$

$$l_2 = |\vec{r}_4 - \vec{r}_2| - l_o = 2|\vec{\rho}_3 + \vec{\rho}_1| - l_o$$

$$l_3 = |\vec{r}_4 - \vec{r}_3| - l_o = 2|\vec{\rho}_1 + \vec{\rho}_2| - l_o$$

$$l_4 = |\vec{r}_2 - \vec{r}_3| - l_o = 2|\vec{\rho}_2 - \vec{\rho}_3| - l_o$$

$$l_5 = |\vec{r}_3 - \vec{r}_1| - l_o = 2|\vec{\rho}_3 - \vec{\rho}_1| - l_o$$

$$l_6 = |\vec{r}_1 - \vec{r}_2| - l_o = 2|\vec{\rho}_1 - \vec{\rho}_2| - l_o \ .$$

Then the potential may be any arbitrary positive definite quadratic form in the l_i's (i = 1, ... , 6), but symmetric with respect to all particles. The most general such potential is:

$$V = \frac{1}{2} V_1(l_1^2 + l_2^2 + l_3^2 + l_4^2 + l_5^2 + l_6^2) + V_2[(l_1 + l_4)(l_2 + l_3 + l_5 + l_6) + (l_2 + l_5)(l_3 + l_6)] + V_3[l_1 l_4 + l_2 l_5 + l_3 l_6]$$

where the first term sums over all sides separately, the second over pairs of adjacent sides, and the third over opposite sides. We note that if only two body forces were involved, V_2 and V_3 would both vanish.

2.2. Normal Modes.

The normal modes $\vec{r}_n^{(i)} = \vec{d}_{ni}\ \varepsilon_i$, $i = 1, \ldots, 6$, are in principle to be chosen so that they are orthonormal (which diagonalizes the kinetic energy):

$$M \sum_{n=1}^{4} \vec{d}_{ni} \cdot \vec{d}_{nj} = \delta_{ij} ;$$

so that they are irrotational:

$$\sum_{n=1}^{4} \vec{d}_{ni} \times \vec{r}_{no} = 0 ;$$

and so that the potential function is diagonalized:

$$V_l(l_i) = V_r(\vec{r}_i) = V_\varepsilon(\varepsilon_i) = \sum_{i=1}^{6} V_i\ \varepsilon_i^2 ,$$

at least to second order, i.e., V is not expressible exactly as a second order expansion in ε_i , however we are interested only in the second order potential. In principle, the higher order potential terms could be obtained as well.

Expressing these results in terms of the $\vec{\rho}_i$'s,

$$\vec{\rho}_\alpha^{(i)} = \vec{b}_{\alpha i}\ \varepsilon_i \qquad \alpha = 1, 2, 3, ;\ \ i = 1, 2, \ldots, 6$$

$$\sum_{\alpha=1}^{3} \vec{b}_{\alpha i} \cdot \vec{b}_{\alpha j} = \frac{1}{4M}\ \delta_{ij}$$

$$\sum_{\alpha=1}^{3} \vec{b}_{\alpha i} \times \vec{\rho}_{\alpha o} = 0 .$$

Thus if we wrote $\vec{b}_{\beta i} \cdot \hat{1}_{\alpha} = b_{\alpha\beta\, i}$, $\sum_i b_{\alpha\beta\, i}\, \varepsilon_i$ may be any arbitrary symmetric matrix in α, β ; and it is easiest to write the normal modes down by inspection and verify that the potential is diagonalized.

$$\begin{pmatrix} \vec{\rho}_1 \\ \vec{\rho}_2 \\ \vec{\rho}_3 \end{pmatrix} = a \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix}$$

$$+ \frac{1}{\sqrt{4M}} \begin{pmatrix} \frac{\varepsilon_1}{\sqrt{3}} - \frac{\varepsilon_2}{\sqrt{2}} + \frac{\varepsilon_3}{\sqrt{6}} & \frac{\varepsilon_6}{\sqrt{2}} & \frac{\varepsilon_5}{\sqrt{2}} \\ \frac{\varepsilon_6}{\sqrt{2}} & \frac{\varepsilon_1}{\sqrt{3}} - \frac{\varepsilon_2}{\sqrt{2}} + \frac{\varepsilon_3}{\sqrt{6}} & \frac{\varepsilon_4}{\sqrt{2}} \\ \frac{\varepsilon_5}{\sqrt{2}} & \frac{\varepsilon_4}{\sqrt{2}} & \frac{\varepsilon_1}{\sqrt{3}} - \frac{2\varepsilon_2}{\sqrt{6}} \end{pmatrix} \begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix}$$

In terms of the ε_i's, we have to first order

$$(l_i) = \frac{\sqrt{2}}{\sqrt{4M}} \begin{pmatrix} \frac{2}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} & \sqrt{2} & 0 & 0 \\ \frac{2}{\sqrt{3}} & \frac{-1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} & 0 & \sqrt{2} & 0 \\ \frac{2}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} & 0 & 0 & \sqrt{2} \\ \frac{2}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} & -\sqrt{2} & 0 & 0 \\ \frac{2}{\sqrt{3}} & \frac{-1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} & 0 & -\sqrt{2} & 0 \\ \frac{2}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} & 0 & 0 & -\sqrt{2} \end{pmatrix} (\varepsilon_i)$$

whence to second order

$$V = \frac{1}{2M} [\varepsilon_1^2(4V_1 + 16V_2 + 4V_3) + (\varepsilon_2^2 + \varepsilon_3^2) \quad (V_1 - 2V_2 + V_3)$$
$$+ (\varepsilon_4^2 + \varepsilon_5^2 + \varepsilon_6^2) (2V_1 - 2V_3)] \quad .$$

Now since we have no a priori knowledge of V_1, V_2, V_3, we may conveniently use:

$$V = \frac{1}{2} [\omega_1^2\varepsilon_1^2 + \omega_2^2(\varepsilon_2^2 + \varepsilon_3^2) + \omega_3^2(\varepsilon_4^2 + \varepsilon_5^2 + \varepsilon_6^2)]$$

where

$$\omega_1 = \sqrt{\frac{1}{M} (4V_1 + 16V_2 + 4V_3)}$$

$$\omega_2 = \sqrt{\frac{1}{M} (V_1 - 2V_2 + V_3)}$$

$$\omega_3 = \sqrt{\frac{1}{M} (2V_1 - 2V_3)}$$

are the angular frequencies of the classical vibration.

The vibrational modes consist of a non-degenerate dilational modes, a doubly-degenerate pair-twisting mode, and a triply degenerate mode in which one side of the tetrahedron shrinks while the opposite expands.

3.0. Quantum Mechanical Vibrational Hamiltonian.

In obtaining the wave functions for the vibrational motion, we will find it convenient to use dimensionless coordinates

let
$$\varepsilon_i = \frac{q_i a \sqrt{4M}}{a_i}$$

$$p_{\varepsilon_i} = \dot{\varepsilon}_i = \frac{a_i p_i}{a \sqrt{4M}}$$

where

$$\alpha_i = \frac{a}{\hbar} \sqrt{4Mw_i}$$

and

$$w_i = \hbar \, \omega_i \quad .$$

Then the vibrational QM Hamiltonian becomes

$$H_{vib} = \frac{1}{2} w_1 \left(\frac{p_1^2}{\hbar^2} + q_1^2 \right) + \frac{1}{2} w_2 \sum_{i=2}^{3} \left(\frac{p_i^2}{\hbar^2} + q_i^2 \right) + \frac{1}{2} w_3 \sum_{i=4}^{6} \left(\frac{p_i^2}{\hbar^2} + q_i^2 \right)$$

and the wave functions Ψ_{vib} satisfying the Schroedinger equation

$$H_{vib} \Psi_{vib} = E_{vib} \Psi_{vib}$$

are

$$\Psi_{vib} = \exp(- \frac{1}{2} \sum_{i=1}^{6} q_i^2) \prod_{i=1}^{6} H_{n_i} (q_i)$$

with eigenvalues

$$E_{vib} = w_1(n_1 + \frac{1}{2}) + w_2(n_2 + n_3 + 1) + w_3(n_4 + n_5 + n_6 + \frac{3}{2})$$

and

$$H_n(\xi) = (-1)^n e^{\xi^2} (\frac{\partial}{\partial \xi})^n e^{-\xi^2}$$

are the usual Hermite polynomials with normalization

$$\int_{-\infty}^{\infty} H_n^2(\xi) e^{-\xi^2} d\xi = \pi^{1/2} 2^n n! \quad .$$

3.1. Rotational-Vibrational Interaction Terms. Complete Hamiltonian.

In order to develop the complete Hamiltonian, even in the lowest order approximation, we require expressions for the internal angular momentum operators $\vec{\pi}$ and the dynamic tensor $\mu^{\alpha\beta}$

$$\vec{\pi} = \sum_{i,j=1}^{6} \vec{\zeta}_{ij} q^i p_j \quad ,$$

where

$$\vec{\zeta}_{ij} = M \sum_{n=1}^{4} \vec{d}_{ni} \times \vec{d}_{nj} = 4M \sum_{\alpha=1}^{3} \vec{b}_{\alpha i} \times \vec{b}_{\alpha j} \quad ,$$

the d's and b's being as previously defined (Sect. II, 2.2):

$$\vec{b}_{\alpha i} = \frac{1}{\sqrt{4M}} \begin{pmatrix} \frac{\hat{i}'}{\sqrt{3}} & \frac{-\hat{i}'}{\sqrt{2}} & \frac{\hat{i}'}{\sqrt{6}} & 0 & \frac{\hat{k}'}{\sqrt{2}} & \frac{\hat{j}'}{\sqrt{2}} \\ \frac{\hat{j}'}{\sqrt{3}} & \frac{\hat{j}'}{\sqrt{2}} & \frac{\hat{j}'}{\sqrt{6}} & \frac{\hat{k}'}{\sqrt{2}} & 0 & \frac{i'}{\sqrt{2}} \\ \frac{\hat{k}'}{\sqrt{3}} & 0 & \frac{-2\hat{k}'}{\sqrt{6}} & \frac{j'}{\sqrt{2}} & \frac{i'}{\sqrt{2}} & 0 \end{pmatrix}$$

$$\vec{\zeta}_{ij} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i'}{2} & \frac{j'}{2} & -k' \\ 0 & 0 & 0 & \frac{i'\sqrt{3}}{2} & \frac{-j'\sqrt{3}}{2} & 0 \\ 0 & \frac{-i'}{2} & \frac{-i'\sqrt{3}}{2} & 0 & \frac{-k'}{2} & \frac{j'}{2} \\ 0 & \frac{j'}{2} & \frac{j'\sqrt{3}}{2} & \frac{k'}{2} & 0 & \frac{-i'}{2} \\ 0 & k' & 0 & \frac{-j'}{2} & \frac{i'}{2} & 0 \end{pmatrix}$$

This matrix possesses the property that $\sum_{i=1}^{6} (\vec{\zeta}_{ij} \times \vec{\zeta}_{ik}) \times \vec{\zeta}_{jk} = 0$ for all i, k, so that the arguments of p. 25 (2) will apply.

$$\vec{\pi} = \vec{\pi}^{o} + \vec{\pi}'$$

where

$$\vec{\pi}^{o} = -\frac{1}{2} [\hat{i}'(q_6p_6 - q_6p_5) + \hat{j}'(q_6p_4 - q_4p_6) + \hat{k}'(q_4p_5 - q_5p_4)]$$

$$\vec{\pi}^{1} = \hat{i}'[q_4(-\frac{p_2}{2} - \frac{\sqrt{3}}{2} p_3) - (-\frac{q_2}{2} - \frac{\sqrt{3}}{2} q^3) p_4]$$

$$+ \hat{j}'[q_5(-\frac{p_2}{2} + \frac{\sqrt{3}}{2} p_3) - (-\frac{q_2}{2} + \frac{\sqrt{3}}{2} q^3)p_5] + \hat{k}'(q_6p_5 - q_5p_6)$$

and we shall regard the terms arising from $\vec{\pi}^1$ as being of higher order since they mix vibration states of different energies.

For the dynamic tensor, we shall find it sufficient to use the zero-order approximation, which is the coordinate independent part of the inertial tensor, and in this case is simply

$$\mu_0^{\alpha\beta} = \mu_0^{\alpha} \, \delta_{\alpha\beta} = \frac{1}{I_0} \, \delta_{\alpha\beta} \text{ , where}$$

$$I_0 = \frac{8}{3} Ma^2 \quad .$$

3.2. Complete Hamiltonian. General Solution.

Upon putting together the expressions for $\mu_0^{\alpha\beta}$, for the internal angular momentum and for the quantum mechanical vibrational Hamiltonian we arrive at the complete zeroth order Hamiltonian:

$$H^0 = \frac{1}{2I_0} (\vec{P} - \vec{\pi}^0)^2 + \frac{1}{2} w_1 \left(\frac{p_1^2}{\hbar^2} + q_1^2 \right) + \frac{1}{2} w_2 \sum_{i=2}^{3} \left(\frac{p_i^2}{\hbar^2} + q_i^2 \right)$$

$$+ \frac{1}{2} w_3 \sum_{i=4}^{6} \left(\frac{p_i^2}{\hbar^2} + q_i^2 \right) \quad ,$$

and for convenience we shall introduce for $\vec{P}$ and $\vec{\pi}^0$ two more convenient operators, i.e., let

$$\vec{P} = \hbar \vec{J}$$

$$\vec{\pi}^0 = \zeta \hbar \vec{L}$$

where $\vec{J}$ is the usual operator for total angular momentum/$\hbar$. $\vec{L}$ corresponds to the usual orbital angular momentum/$\hbar$ operator, except that it operates on q_4, q_5, q_6 instead of x, y, z.

ζ is a constant = - 1/2.

We then obtain

$$H^o = \frac{\hbar^2}{2I_o} (\vec{J} - \zeta \vec{L})^2 + \frac{w_1}{2} \left(\frac{p_1^2}{\hbar^2} + q_1^2 \right) + \frac{w_2}{2} \sum_{i=2}^{3} \left(\frac{p_i^2}{\hbar^2} + q_i^2 \right)$$

$$+ \frac{w_3}{2} \sum_{i=4}^{6} \left(\frac{p_i^2}{\hbar^2} + q_i^2 \right) .$$

It will turn out that $\vec{L}^2$ has eigenvalue $L(L+1)$ where L is a good quantum number, and that stationary state wave functions are therefore eigenvalues of $\vec{J} \cdot \vec{L}$.

If (note the change in the use of n_i)

n_1 = excitation level of vibration state q_1 with excitation energy w_1.

n_2 = excitation level of vibration states q_2, q_3 with excitation energy w_2.

n_3 = excitation level of vibration states q_4, q_5, q_6 with excitation energy w_3.

$$w_o = \frac{\hbar^2}{I_o} .$$

Then the excitation energy of any state is given by

$$E = w_o \left[\frac{1}{2} J(J+1) + \frac{1}{2} {}^2 L(L+1) - \zeta (\vec{J} \cdot \vec{L}) \right] + n_1 w_1 + n_2 w_2 + n_3 w_3 .$$

To determine the excitation energy of allowed states, we need to know the parameters J, L, $(\vec{J} \cdot \vec{L})$, n_1, n_2, n_3 for all allowed stated in which we are interested, and to fix the values of energies w_o, w_1, w_2, w_3 by identifying four known excitation levels.

4.0. Allowed Levels. Group Properties.

We can determine the above parameters for allowed states by using the group theoretical method developed in Part I. In this case the subgroup of rotations R coincides with the permutation group P which is isomorphic with the abstract group P_4 of permutations of four objects.

We shall employ the standard "cycle" notation for the elements of P_4:

E is the identity element.

(12) means a simple permutation of objects 1 and 2.

(123) = (12)(23) or the permutation (23) followed by (12) (operators are considered to operate to the right), under which $1 \rightarrow 2$, $2 \rightarrow 3$, $3 \rightarrow 1$.

An element is invariant to cyclic permutation of the symbols within any one cycle:

$$(1234) = (12)(23)(34) = (2341) = (23)(34)(12) \quad \text{etc.}$$

All elements with the same cycle structure belong to the same class, since a similarity transformation relabels the symbols but cannot change the cycle structure.

The irreducible representations of the abstract group P_4 are denoted by the symmetry pattern to which the basis functions for the representation belong. There are five such:

(1111), (211), (22), (31), (4).

Of these, the first is completely symmetric in the four permuted objects; the last completely anti-symmetric; and (31), for instance, is the group of transformations on functions anti-symmetric in three of the permuted objects, symmetric between that set of three and the fourth object.

The primitive characterization of P_4 is:

Class	Number of elements	h(S)	(1111)	(211)	(22)	(31)	(4)
E	1		1	3	2	3	1
(12)	6		1	1	0	-1	-1
(12)(34)	3		1	-1	2	-1	1
(123)	8		1	0	-1	0	1
(1234)	6		1	-1	0	1	-1

4.1. Calculation of $n^E(\alpha)$.

For the first excited vibrational states, the wave functions transform like the coordinates q_i or ε_i which are linear combinations of the quantities $l_1, l_2, \ldots, l_6$, the perturbations in lengths of sides of the tetrahedron. Under the operations of the group P, the l's simply permute among themselves, and we can find the irreducible representations to which the q_i belong by seeing what irreducible representations of P_4 are induced in the six-dimensional representation of P_4 by $U^l_{ij}(S)$

$$S(l_i) = \sum_{j=1}^{6} U^l_{ij}(S)\, l_j \; .$$

Consider the standard configuration of Fig. 1. $U^l_{ij}(S)$ is a permutation matrix and thus has elements which are either 0 or 1, each row or column having only a single element different from zero. Thus $\chi^l(S)$ is equal to the number of l_i's which are unchanged in the permutation and we have at once:

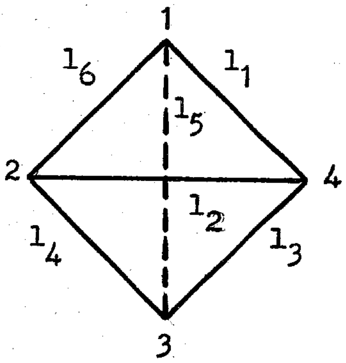


Fig. 1

$$\chi^{1}(E) = 6$$

$$\chi^{1}(12) = 2$$

$$\chi^{1}(123) = 0$$

$$\chi^{1}(12)(34) = 2$$

$$\chi^{1}(1234) = 0 \quad .$$

Applying the equation for summation over group characters:

$$n^{1}(\alpha) = \frac{1}{h} \sum_{\text{classes}} h(S)\, \chi^{*}_{\alpha}(S)\, \chi^{1}(S) \quad ,$$

we find

$$n^{1}(1111) = n^{1}(211) = n^{1}(22) = 1$$

$$n^{1}(31) = n^{1}(4) = 0 \quad .$$

Thus there is a

1 dimensional representation (1111),
2 dimensional representation (22),
3 dimensional representation (211).

Looking at the q^{i}'s we find belonging to vibrational energy w_1, a single q_1 ; to w_2 , two states q_2, q_3, and to w_3, three states q_4, q_5, q_6; which therefore belong to the irreducible representations 1111, 22, 211, respectively.

We would obtain the same results if instead of using the l's as basis vectors the representation, we used the q_i's, themselves. Thus from the defining equations for the ε_i (and hence the q_i), sec. 2.2, we see that

$$q_1 \text{ transforms as } \frac{x^2 + y^2 + z^2}{\sqrt{3}} ;$$

$$q_3, q_2 \text{ transform as } \frac{2z^2 - x^2 - y^2}{\sqrt{3}}, \frac{x^2 - y^2}{\sqrt{2}}, \text{ resp.;}$$

$$(q_4, q_5, q_6) \text{ transform as } (yz, xz, xy) \text{ , resp.;}$$

and since in the group of transformations P , (x, y, z) go into any permutation of (x, y, z), with the same sign or with two negative signs, q_1 is invariant, and since xyz → xyz ; (yz, xz, xy) transform exactly as (x, y, z), and so

$$q_4, q_5, q_6 \text{ transform as } (x, y, z) .$$

To make use of this, however, we used an explicit representation for the elements of P. It is given in Appendices II and III.

Using the explicit representation of P in the space of the q_i , we can find $n^E(\alpha)$ for the higher excited states as well.*

---

* For the states $2w_2$, $2w_3$ we use as basis vectors q_2^2, q_2q_3, q_3^2 and $q_4^2, q_5^2, q_6^2, q_4q_5, q_4q_6, q_5q_6$, respectively; find the characters of the classes of the induced representation and then use the character summation to find $n^E(\alpha)$.

For the state $3w_2$, we similarly use $q_2^3, q_2^2q_3, q_2q_3^2, q_3^3$.

For combination states $n_2w_2 + n_3w_3$, we note that $U^{(n_2w_2)} \times U^{(n_3w_3)}$ induces on the space of product functions a reducible representation with characters $\chi^{(n_2w_2)}(S)\ \chi^{(n_3w_3)}(S)$, and apply the character summation to find $n^E(\alpha)$.

We note that the symmetry is indifferent to the excitation level n_1 of the dilatational vibration q_1, and so give the values of $n^E(\alpha)$ as a function of n_2 and n_3 only. In addition we include the value of the internal angular momentum quantum number L. We consider states $0 \leq n_2 \leq 3$, $0 \leq n_3 \leq 2$, $0 \leq n_2 + n_3 \leq 3$.

$E' = n_2w_2 + n_3w_3$	L	$n^E_{(1111)}$	$n^E_{(211)}$	$n^E_{(22)}$	$n^E_{(31)}$	$n^E_{(4)}$
0	0	1	0	0	0	0
w_2	0	0	0	1	0	0
w_3	1	0	1	0	0	0
$2w_2$	0	1	0	1	0	0
$w_2 + w_3$	1	0	1	0	1	0
$2w_3$	0	1	0	0	0	0
$2w_3$	2	0	1	1	0	0
$3w_2$	0	1	0	1	0	1
$2w_2 + w_3$	1	0	1	0	1	0
$w_2 + 2w_3$	0	0	0	1	0	0
$w_2 + 2w_3$	2	1	1	1	1	1

4.2. Calculation of $n^{\pm J}(\alpha)$.

Here we make use of the known characters of the irreducible representations $D^{\pm}_J$ of the rotation group. All rotations through the total angle θ belong to two classes: proper rotations through θ (no inversion) and improper rotations through θ (with inversion).

Denoting these by (θ, ϑ); $\vartheta = 0, 1$ for proper, improper rotations

$$\chi^{J\pm}(\theta,\vartheta) = (\pm 1)^{\vartheta} \quad \sin((J + 1/2)\, \theta)/ \sin \frac{\theta}{2}$$

$$\chi^{J\pm}(0,\vartheta) = (\pm 1)^{\vartheta} \; (2J + 1) \;.$$

By referring to the standard configuration

and the inverted configuration, in Fig. 2,

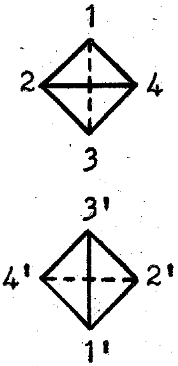


Fig. 2

we can find the rotation corresponding to any permutation and obtain:

Class(S)		θ	$\chi^{0\pm}(S)$	$\chi^{1\pm}(S)$	$\chi^{2\pm}(S)$	$\chi^{3\pm}(S)$	$\chi^{4\pm}(S)$	$\chi^{5\pm}(S)$
E	0	0	1	3	5	7	9	11
(12)	1	π	± 1	∓ 1	± 1	∓ 1	± 1	∓ 1
(12)(34)	0	π	1	-1	1	-1	1	- 1
(123)	0	$\frac{2\pi}{3}$	1	0	-1	1	0	- 1
(1234)	1	$\frac{\pi}{2}$	± 1	± 1	∓ 1	∓ 1	± 1	± 1

and the $n^{J\pm}(\alpha)$ are:

J	0^+	0^-	1^+	1^-	2^+	2^-	3^+	3^-	4^+	4^-	5^+	5^-
n(1111)	1	0	0	0	0	0	0	1	1	0	0	0
n(211)	0	0	0	1	1	0	1	1	1	1	1	2
n(22)	0	0	0	0	1	1	0	0	1	1	1	1
n(31)	0	0	1	0	0	1	1	1	1	1	2	1
n(4)	0	1	0	0	0	0	1	0	0	1	0	0

We note that the lowest state containing (1111) is 0^+, (211) is 1^-, (22) is 2^+, and the lowest purely rotationally excited state is 3^-.

5.0. Computation of Energy Levels.

Having found the $n^E(\alpha)$ and $n^{J\pm}(\alpha)$ we could proceed by the method of Part I, sec. 4.2 to find the energy levels of the Hamiltonian neglecting the $\vec{J} \cdot \vec{L}$ term, but we should then have to compute wave functions and combinations which diagonalize the $\vec{J} \cdot \vec{L}$ term in order to obtain the complete energy expression.

Instead we use the following procedure in which we combine tha angular function with the $n_3 w_3$ vibration state first, and then combine the resulting state with the $n_2 w_2$ state to form an invariant under P and last add the $n_1 w_1$ state which does not alter the invariance.

The Hamiltonian we used is expressed as:

$$H^o = \frac{1}{2} w_o(\vec{J} - \zeta \vec{L})^2 + \frac{1}{2} w_1 \left(\frac{p_1^2}{\mu^2} + q_1^2 \right)$$

$$+ \frac{1}{2} w_2 \sum_{i=2}^{3} \left(\frac{p_i^2}{\mu^2} + q_i^2 \right) \ \frac{1}{2} w_3 \sum_{i=4}^{6} \left(\frac{p_i^2}{\mu^2} + q_i^2 \right) ,$$

and the excitation energy of a state is

$$E = w_o \frac{1}{2} [J(J+1) + \frac{1}{2} \zeta^2 L(L+1) - \zeta (\vec{J} \cdot \vec{L})] + n_1 w_1 + n_2 w_2 + n_3 w_3$$

and we need to determine the permissible combinations of J, L, $\vec{J} \cdot \vec{L}$, n_1, n_2, n_3, that define an allowed state.

First we note that L is an angular momentum operator which operates on the coordinates q_4, q_5, q_6, of the triply degenerate state;

$$\vec{L} = L_x\hat{i}' + L_y\hat{j}' + L_z\hat{k}'$$

$$L_x = q_5p_6 - q_6p_5$$

$$L_y = q_6p_4 - q_4p_6$$

$$L_z = q_4p_5 - q_5p_4$$

$\hat{i}'$, $\hat{j}'$, $\hat{k}'$ are body axes, corresponding to body coordinates x, y, z so that $\hat{i}'$, $\hat{j}'$, $\hat{k}'$ rotate with the configuration.

For first excited states of q_4, q_5, q_6, we form the combinations $v_1^1\ \Psi_o$, $v_1^o\ \Psi_o$, $v_1^{-1}\ \Psi_o$, where Ψ_o is the ground state wave function and will be understood hereafter as a factor of all vibration wave functions, and

$$v_1^1 = -\ 2^{-1/2}(q_4 + iq_5)$$

$$v_1^o = q_6$$

$$v_1^{-1} = 2^{-1/2}(q_4 - iq_5)\ .$$

Then v_1^1 , v_1^o , v_1^{-1}, are wave functions for $n_3 = 1$ and simultaneously are eigenfunctions of L and $j = L_z$ with $L = 1$ and $j = 1, 0, -1$, respectively.

For second excited state of q_4, q_5, q_6 , we can find similar combinations

$$v_o^o = q_4^2 + q_5^2 + q_6^2 - \frac{3}{2}$$

which has $L = 0$ and belongs to the (1111) representation of P_4, and

$$v_2^o = \frac{(v_1^o)^2 + v_1^1\ v_1^{-1}}{\sqrt{3}}$$

$$\frac{1}{\sqrt{2}}\ (v_2^2 + v_2^{-2}) = \frac{1}{\sqrt{2}}\ [(v_1^1)^2 + (v_1^{-1})^2]$$

which have L = 2 and belongs to the (22) representation of P_4, and

$$v_2^1 = \sqrt{3}\, v_1^1\, v_1^o$$

$$\frac{1}{\sqrt{2}} (v_2^2 - v_2^{-2}) = \frac{\sqrt{3}}{2} \quad (v_1^1)^2 - (v_1^{-1})^2$$

$$- v_2^{-1} = \sqrt{3}\, v_1^{-1}\, v_1^o$$

which have L = 2 and belong to the (211) representation of P_4.

The notation of the v_L^j is the usual one for an angular wave function for total angular momentum L and z component j (in units of $\hbar$). Hence if

$$L_+ = L_x + iL_y$$

$$L_- = L_x - iL_y \quad ,$$

we have

$$L_+ v_L^j = \sqrt{(L - j)(L + j + 1)} \quad v_L^{j+1}$$

$$L_- v_L^j = \sqrt{(L + j)(L - j + 1)} \quad v_L^{j-1}$$

$$L_z v_L^j = j\, v_L^j \quad .$$

Now in the Hamiltonian there occurs $\vec{L} \cdot \vec{J}$

$$\vec{L} \cdot \vec{J} = L_x J'_x + L_y J'_y + L_z J'_z$$

where the primes on J'_x, J'_y, J'_z indicate operators for components of angular momentum on the rotating body axes (identical with S' operators of Appendix I), and with

$$J'_+ = J'_x + iJ'_y$$

$$J'_- = J'_x - iJ'_y$$

we have

$$\vec{L} \cdot \vec{J} = \frac{1}{2} (L_+ \, J'_- + L_- \, J'_+) + L_z \, J'_z \, .$$

Acting on the symmetric top wave functions $Y^{km}_{J\pm}$ (Eq. A1.19)

$$J'_+ \, Y^{km}_J = \sqrt{(J + k)(J - k + 1)} \;\; Y^{k-1,m}_J$$

$$J'_- \, Y^{km}_J = \sqrt{(J - k)\;(J + k + 1)} \;\; Y^{k+1,m}_J$$

$$J'_2 \, Y^{km}_J = k \; Y^{km}_J \quad .$$

Thus when acting on a product wave function $v^j_L \, Y^{km}_J$, the operator $\vec{L} \cdot \vec{J}$ can simultaneously raise j and k, lower both, or leave them unchanged.

Note now that any eigenfunction of $(\vec{J} - \varsigma \vec{L})^2$ which is also simultaneously eigenfunction of J^2 and L^2 is an eigenfunction of $\vec{J} \cdot \vec{L}$ and hence an eigenfunction of a (perhaps fictitious) angular momentum $\vec{I} = \vec{J} - \vec{L}$. (The minus sign is chosen here because $\vec{J} \cdot \vec{L}$ conserves $j - k$ instead of $j + k$, and so with this choice, $I_z = j - k$ commutes with $\vec{J} \cdot \vec{L}$.)

Then by the vector addition rule for angular momenta we obtain

$$\vec{J} \cdot \vec{L} = \frac{1}{2} J(J + 1) + \frac{1}{2} L(L + 1) - \frac{1}{2} I(I + 1).$$

In addition to the quantum number I of the pseudo angular momentum I we introduce a parity which is the product of the parity of J and that of L. (The parity of L is $(-1)^{n_3}$.)

Then $I_\pm$ has a mathematical if not a physical interpretation: under the rotational subgroup P , the wave function for the rotation +

the w_3 vibration transforms like an angular wave function belonging to total angular momentum and parity $I_{\pm}$.

An allowed state is formed by combining the function which transforms like $I_{\pm}$ with the w_2 vibrational wave function to form a total wave function which belongs to the (1111) representation of P_4 . We disregard the value of n_1 in this procedure since q_1 belongs to (1111) and never affects the symmetry of a wave function.

5.1. Determination of Allowed States.

(1) Pure Rotational States: $n_2, n_3 = 0, 0$.

The only $J\pm$ states which contain (1111) are 3^- and 4^+ . Hence the only states with $n_2 = n_3 = 0$ are $J = 0^+, 3^-, 4^+$.

(2) Singly Excited Vibrational States: $n_2 + n_3 = 1$.

(a) $n_2, n_3 = 1, 0$.

$J = 2^{\pm}, 4^{\pm}, 5^{\pm}$ are possible, since to form an invariant we must choose a set of angular wave functions belonging to the (22) representation.

(b) $n_2, n_3 = 0, 1$.

$J = 1^-, 2^+, 3^{\pm}, 4^{\pm}, 5^{\pm}, \ldots$ are possible since there are wave functions of these $J\pm$ values which belong to (211) representation.

Here, however, $L = 1$ and we need to determine I. We note that the states of $n_3 = 1$ transform under P exactly like angular functions for $J = 1^-$. Thus more exactly, $L = 1^-$ and for a given $J\pm$, we can have

$$I = (J + 1)_{\mp} , \qquad J_{\mp} , \qquad (J - 1)_{\mp} .$$

However the total wave functions transform under P like an angular function for angular momentum $I_{\pm}$, hence we must have

$$I = 0^{+},\ 3^{-},\ 4^{+},$$

and so the following values are possible:

J	1^{-}	2^{+}	3^{+}	3^{-}	4^{+}	4^{-}	...
I	0^{+}	3^{-}	3^{-}	4^{+}	3^{-}	4^{+}	

(3) <u>Second Excited Vibrational States</u>: $n_2 + n_3 = 2$.

(a) $n_2, n_3 = 2, 0$.

States of $2w_2$ belong either to (1111) or (22), so for

(1111) vibrational states $J = 0^{+}, 3^{-}, 4^{+}, \ldots$

(22) vibrational states $J = 2^{\pm}, 4^{\pm}, \ldots$.

The degeneracy in the 4^{+} state is unresolved.

(b) $n_2, n_3 = 1, 1$.

States of $w_2 + w_3$ belong either to (211) or to (31).

Hence $J = 1^{\pm}, 2^{\pm}, 3^{\pm}, 3^{\pm}, \ldots$ are possible. However, $L = 1^{-}$ here, and so we first combine the $L(w_3)$ functions with the $J\pm$ functions to form $I\pm$, and then combine the I functions with the w_2 functions to form a total wave function belonging to (1111).

The intermediate $I\pm$ here will have to belong to (22). Hence for a given $J\pm$,

$$I = 2^{\pm}, 4^{\pm}, \ldots$$

$$I = (J - 1)_{\mp},\ J_{\mp},\ (J + 1)_{\mp} \quad .$$

Possible combinations are:

J	$1^{\pm}$	$2^{\pm}$	$3^{\pm}$	$3^{\pm}$	...
I	$2^{\mp}$	$2^{\mp}$	$4^{\mp}$	$2^{\mp}$	

(c) $n_2, n_3 = 0, 2.$

States of $2w_2$ may belong to (1111) with $L = 0^+$; or to (211) or (22) with $L = 2^+$:

(1111) states: here $L = 0^+$, $I = J$, $J = 0^+, 3^-, 4^+, \ldots$

(211), (22) states: here $L = 2^+$ and for $J\pm$,

$$I = (J - L)^{\pm},\ (J - 1)^{\pm},\ J\pm,\ (J + 1)^{\pm},\ (J + 2)^{\pm}$$

$$I = 0^+, 3^-, 4^+, \ldots$$

Possible combinations are:

J	1^-	2^+	2^+	2^-	3^+	3^-	...
I	3^-	4^+	0^+	3^-	4^+	3^-	

Complete wave functions for all of the above states (except those with $n_2 + n_3 = 2$, $J > 2$) are given in Appendix IV.

(4) <u>Third Excited Vibrational Levels</u>: $n_2 + n_3 = 3.$

(a) $n_2, n_3 = 3, 0.$

States of $3w_2$ belong to (1111), (22), or (4).

$$J = 0^{\pm}, 2^{\pm}, 3^{\pm}, 4^{\pm}, \ldots .$$

(b) $n_2, n_3 = 2, 1.$

States of $2w_2$ belong to (1111) or (22). $L = 1^-$ here, so for a given $J\pm$,

$$I = (J - 1)_{\mp} , J_{\mp} , (J + 1)_{\mp}$$

$$I = 0^{+}, 2^{\pm}, 3^{-}, 4^{+}, 4^{\pm} .$$

Possible combinations are:

J	1^{+}	1^{-}	1^{-}	...
I	2^{-}	2^{+}	0^{+}	

(c) $n_2, n_3 = 1, 2.$

States of $2w_3$ belong to (1111) with $L = 0^{+}$, or to (211) or (22) with $L = 2^{+}$,

with $L = 0^{+}, I = J, J = 2^{\pm}, 4^{\pm} , \ldots$

with $L = 2^{+}, J \pm$

$$I = (J - 2)_{\pm} , \ldots , (J + 2)_{\pm}$$

$$I = 2^{\pm} , 4^{\pm} , \ldots .$$

Possible states with $L = 2$ are:

J	$0^{\pm}$	$1^{\pm}$	$2^{\pm}$	$2^{\pm}$
I	$2^{\pm}$	$2^{\pm}$	$4^{\pm}$	$2^{\pm}$.

The above states are sufficient to compute all energy levels whose excitation energy is less than 16 Mev.

5.2. Computed Energy Levels.

Table I gives the value of $n_1, n_2, n_3, J\pm, L\pm, \vec{J} \cdot \vec{L}$ (and redundantly $I_{\pm}$) for the lower excited states of O^{16} on the α-particle model, and the resulting energy expressions:

$$E = n_1w_1 + n_2w_2 + n_3w_3 + w_o[\tfrac{1}{2} J(J + 1) + \tfrac{1}{8} L(L + 1) + \tfrac{1}{2} \vec{J} \cdot \vec{L}]$$

or

$$E = n_1w_1 + n_2w_2 + n_3w_3 + w_o[\tfrac{3}{4} J(J + 1) + \tfrac{3}{8} L(L + 1) - \tfrac{1}{4} I(I + 1)].$$

Also included in Table I are quantitative determinations of the energies following the two methods of identification suggested by Dennison [6]. Energies used in the identification are indicated in parentheses. All states whose energy is less than 16 Mev under either method of identification have been included.

Tentative correlations with observed energy levels (uncertain levels are set off in brackets) whose J and parity are known are also given in Table I. The observed energy levels up to 13.65 Mev are tabulated in Table II, together with their correlations on the two identification schemes. Unobserved levels predicted on both schemes are listed in Table III.

5.3. Comparison of the Two Identification Schemes.

Using identification (b) it is possible to fit all levels within 1 Mev and most levels considerably more accurately.

Using identification (a) it is impossible to fit the 12.95 Mev $J = 2^-$ level within 2.3 Mev, or to fit the 13.24 Mev $J = 4^+$ level within 2.7 Mev. Further, if the state at 13.65 turns out to have $J = 2^-$, then it cannot be fitted within 2 Mev and if there is a 0^+ state at ~ 12.5 Mev, it cannot be fitted within 1 Mev.

Thus the older identification (b) is better able to fit the observed energies up to 13.65 Mev. However, the equivalence theory for neutrons and protons requires the correspondence of four levels in O^{16} to the four known levels (0 to .391 Mev) in N^{16}. Since N^{16} has isotopic spin $T = 1$ ($T_z = 1$) the corresponding O^{16} levels must have

$T = 1$ ($T_z = 0$), but since α-particles have intrinsic $T = 0$, these levels could not appear on the α-particle model. Ajzenberg and Lauritsen* [7] find that these levels (the lowest has $J = 2^-$) should appear at energies 12.95 through 13.34 Mev in O^{16}.

Thus the lack of the 12.95 Mev ($J = 2^-$), the 13.24 Mev ($J = 4^+$) and perhaps the $J = 13.65$ level should be regarded as evidence for rather than against identification (a).

Further in the range 0 - 12.5 Mev, identification (a) predicts only five unobserved levels whereas identification (b) predicts ten (both being figured on the basis that there exists 0^+ and 2^+ levels at ~ 12.5 Mev, and disregarding the possible level between 7.12 Mev and 9.58 Mev).

Thus from energy level considerations alone, it appears that identification (a) is favored, but the evidence is not overwhelming.

5.4. Inversion Doubling.

In the above calculation, we have omitted the effect of inversion doubling, which must theoretically arise from the symmetry of the potential with respect to inversion. In the pair twisting mode of energy w_2, the possibility of inversion occurs. As a result, the w_2 states of positive parity should be elevated relative to those of negative parity. However according to Dennison [6], the difference should amount to only several Kev and may be neglected.

---

* Correcting the atomic mass difference for the $n - H^1$ mass difference (.781 Mev) and a coulomb energy difference (3.46 Mev, based upon a uniform charge distribution of radius $1.45\ A^{1/3} \times 10^{-13}$ cm).

TABLE I. Energy Levels of 0^{16} On The α-particle Model.

n_1	n_2	n_3	J±	L±	I±	$\vec{J}\cdot\vec{L}$	E	Identification(a) E_{calc}(Mev)	$E_{obs.}$	Identification(b) E_{calc}(Mev)	$E_{obs.}$
0	0	0	0+				0	0	0+=0	0	0+=0
0	0	0	3−				$6w_o$	(6.14)	3−=6.14	(6.14)	3−=6.14
0	0	0	4+				$10w_o$	10.25	4+=10.36	10.25	4+=10.36
1	0	0	0+				w_1	(6.06)	0+=6.06	(6.06)	0+=6.06
1	0	0	3−				w_1+6w_o	12.20	3−=11.62	12.20	3−=11.62
0	1	0	2±				w_2+3w_o	(9.84)	2+=9.84	(6.91)	2+=6.91
0	1	0	4±				w_2+10w_o	17.00		14.07	4+=13.24
0	0	1	1−	1−	0+	2	$w_3+9w_o/4$	(7.01)	1−=7.12	(7.12)	1−=7.12
0	0	1	2+	1−	3−	-2	$w_3+9w_o/4$	(7.01)	2+=6.91	7.12	
0	0	1	3−	1−	4+	-3	$w_3+19w_o/4$	9.57		9.68	
0	0	1	3+	1−	1−	1	$w_3+27w_o/4$	11.61		11.72	
0	0	1	4−	1−	4+	1	$w_3+43w_o/4$	15.71		15.82	
0	0	1	4+	1−	3−	5	$w_3+51w_o/4$	17.75		17.86	
2	0	0	0+				$2w_1$	12.12	0+=11.25	12.12	[0+=12.5+]
0	2	0	0+				$2w_2$	13.54	[0+=12.5+]	7.68	
0	2	0	2±				$2w_2+3w_o$	16.61		10.75	2+=9.84
0	0	2	0+	0+	0+	0	$2w_3$	9.42		9.64	
0	0	2	1−	2+	3−	-2	$2w_3+3w_o/4$	10.19	1−=9.58	10.41	
0	0	2	2+	2+	4+	-4	$2w_3+7w_o/4$	11.21	2+=11.51	11.93	2+=11.51

TABLE I. continued

								Identification(a)		Identification(b)	
n_1	n_2	n_3	J±	L±	I±	$\vec{J}\cdot\vec{L}$	E	E_{calc}(Mev)	$E_{obs.}$	E_{calc}(Mev)	$E_{obs.}$
0	0	2	2−	2+	3−	0	$2w_3+15w_o/4$	13.26	2−=12.51	13.48	[2−=13.65]
1	1	0	2±				$w_1+w_2+3w_o$	15.90		12.97	2−=12.95
1	0	1	1−	1−	0+	2	$w_1+w_3+9w_o/4$	13.07	1−=13.09	13.18	1−=12.43
1	0	1	2+	1−	3−	−2	$w_1+w_3+9w_o/4$	13.07	[2+=12.5+]	13.18	
0	1	1	1±	1−	2∓	−1	$w_2+w_3+3w_o/4$	12.24	1−=12.24	9.43	1−=9.58
0	1	1	2±	1−	2∓	1	$w_2+w_3+15w_o/4$	15.30		12.49	2−=12.51[2+=12.5+]
0	1	1	3±	1−	4∓	−3	$w_2+w_3+22w_o/4$	17.09		14.28	
0	3	0	0±				$3w_2$	20.31		11.52	0+=11.25
1	2	0	0+				w_1+2w_2	19.60		13.74	
0	3	0	2±				$3w_2+3w_o$	23.28		14.59	
0	2	1	1±	1−	2∓	−1	$2w_2+w_3+3w_o/4$	19.01		13.27	1−=13.09
0	2	1	1−	1−	0+	2	$2w_2+w_3+9w_o/4$	20.55		14.80	
0	2	1	2+	1−	3−	−2	$2w_2+w_3+9w_o/4$	20.55		14.80	
0	1	2	0±	2+	2∓	0	$w_2+2w_3+3w_o/4$	16.96		14.25	

TABLE II. Identification of Known Levels.

		Identification (a)				Identification (b)			
E_{obs}	J p	E_{calc}	n_1	n_2	n_3	E_{calc}	n_1	n_2	n_3
0	0+	0	0	0	0	0	0	0	0
6.05^a	0+	(6.06)	1	0	0	(6.06)	1	0	0
6.14^a	3-	(6.14)	0	0	0	(6.14)	0	0	0
6.91^a	2+	(7.01)	0	0	1	(6.91)	0	1	0
7.12^a	1-	(7.01)	0	0	1	(7.12)	0	0	1
(8.6)									
9.58	1-	10.19	0	0	2	9.43	0	1	1
9.84^a	2+	(9.84)	0	1	0	10.75	0	2	0
10.36	4+	10.25	0	0	0	10.25	0	0	0
(11.10)									
11.25	0+	12.12	2	0	0	11.52	0	3	0
11.51	2+	11.21	0	0	2	11.43	0	0	2
11.62	3-	12.20	1	0	0	12.20	1	0	0
12.43	1-	12.24	0	1	1	13.18	1	0	1
12.51	2-	13.26	0	0	2	12.49	0	1	1
(12.5+)	0+	[13.54	0	2	0]	[12.12	2	0	0]
(12.5+)	2+	[13.07	1	0	1]	[12.49	0	1	1]
12.95	2-	no state ≤ 15.3				12.97	1	1	0
13.09^b	1-	13.09	1	0	1	13.27	0	2	1
13.24	4+	no state ≤ 17.0				14.07	0	1	0
13.65^c	(1+2-)	J=1+ 12.29	0	1	1	J=1+ 13.27	0	2	1
		no 2-state ≤	15.90			J=2- 13.48	0	0	2

Notes: a. Energies from Ajzenberg and Lauritsen [7] .

b. Angular momentum from Schardt, Fowler and Lauritsen [8].

c. Kraus [9].

Reference for all other energies and angular momenta is Bittner and Moffat [10].

TABLE III. Unobserved Levels.

Identification (a)					Identification (b)				
E	J±	n_1	n_2	n_3	E	J±	n_1	n_2	n_3
9.42	0+	0	0	2	6.91	2-	0	1	0
9.57	3-	0	0	1	7.12	2+	0	0	1
9.84	2-	0	1	0	7.68	0+	0	2	0
11.61	3+	0	0	1	9.43	1-	0	1	1
12.24	1+	0	1	1	9.64	0+	0	0	2
					9.68	3-	0	0	1
					10.41	1-	0	0	2
					10.75	2-	0	2	0
					11.52	0-	0	3	0
					11.72	3+	0	0	1

PART III. LIFETIMES OF THE LOWER EXCITED STATES

1. Computation of Mean Lives.

In this section we compute on the α-model the mean lives of the four lowest excited states of O^{16}. For three of these states, namely, the 0^+, 3^-, 1^- states, the identification is independent of which of the two identification schemes (a) or (b) is used. For the fourth, the 2^+ state, the two schemes differ. Hence the lifetimes are computed for the five cases:

Measured Energy (Mev)	Identification	State	Assumed Energy (Mev)
6.06	(a) or (b)	$(1, 0, 0, 0^+)$	6.06
6.14	(a) or (b)	$(0, 0, 0, 3^-)$	6.14
6.91	(a)	$(0, 0, 1, 2^+)$	7.01
	(b)	$(0, 1, 0, 2^+)$	6.91
7.12	(a)*or (b)	$(0, 0, 1, 1^-)$	7.12*

* on identification (a) this energy should be 7.01 Mev, but the small difference is immaterial to the calculations.)

The 3^- to ground, 2^+ to ground, 1^- to ground transitions, which occur by single quantum emission, will be treated first. Then the 0^+ to ground pair production and 2-photon processes will be considered separately.

2.0. Coordinate System.

We shall now express the coordinate system in terms of which all future calculations will be carried out. Let

$\hat{i}, \hat{j}, \hat{k}$	be a right-handed set of unit vectors of fixed cartesian axes.
X, Y, Z	are coordinates of the center of mass in the $\hat{i}, \hat{j}, \hat{k}$, system.
$\hat{i}', \hat{j}', \hat{k}'$	are a set of axes rotated from the $\hat{i}, \hat{j}, \hat{k}$, axes, and constituting body axes for the configuration.
$\phi, \theta, \Psi(\wp)$	are Euler angles (and an inversion operator) describing a rotation from $\hat{i}', \hat{j}', \hat{k}'$ to $\hat{i}, \hat{j}, \hat{k}$: the inversion, if it occurs, will be regarded as preceding the rotation.
Γ	is to be regarded as a shorthand notation for $\phi, \theta, \Psi(\wp)$. Γ with subscripts, primes, etc. will denote other rotations.

The Euler angle convention which is followed here is that of Appendix I on Generalized Spherical Harmonics: In terms of rotations about body axes ($\hat{i}', \hat{j}', \hat{k}'$), a rotation Γ or ϕ, θ, Ψ is one in which the coordinate axes rotate first through Ψ about $\hat{k}'$, second through θ about $\hat{j}'$, third through ϕ about $\hat{k}'$.

Γ's obey right-handed group multiplication: a rotation Γ_1 followed by a rotation Γ to produce a total rotation of Γ_2 is represented by

$$\Gamma_2 = \Gamma_1 \Gamma .$$

$Y^{km}_{J\underline{\pm}}(\Gamma)$	are angular functions obeying the right-handed group property

$$Y^{km}_{J\underline{\pm}}(\Gamma_2) = \sum_{h=-J}^{J} Y^{kh}_{J\underline{\pm}}(\Gamma_1)\, Y^{hm}_{J\underline{\pm}}(\Gamma) .$$

Completing the definition of coordinates, we let:

$q_1, \dots , q_6$ be vibrational coordinates.

Then $X, Y, Z, \Gamma, q_1, \dots , q_6$ are a complete set of coordinates. We shall always disregard the center of mass coordinates, X, Y, Z.

$\vec{r}_1, \dots , \vec{r}_4$ are positions of the particles 1, 2, 3, 4, given by

$$\vec{r}_1 = a \left\{ \left(1 + \frac{q_1}{\alpha_1}\right) \frac{\hat{i}' - \hat{j}' - \hat{k}'}{\sqrt{3}} + \frac{q_2}{\alpha_2} \frac{-\hat{i}' - \hat{j}'}{\sqrt{2}} + \frac{q_3}{\alpha_2} \frac{\hat{i}' - \hat{j}' + 2\hat{k}'}{\sqrt{6}} \right.$$

$$\left. + \frac{q_4}{\alpha_3} \frac{-\hat{j}' - \hat{k}'}{\sqrt{2}} + \frac{q_5}{\alpha_3} \frac{-\hat{i}' + \hat{k}'}{\sqrt{2}} + \frac{q_6}{\alpha_3} \frac{-\hat{i}' + \hat{j}'}{\sqrt{2}} \right\}$$

$$\vec{r}_2 = a \left\{ \left(1 + \frac{q_1}{\alpha_1}\right) \frac{-\hat{i}' + \hat{j}' - \hat{k}'}{\sqrt{3}} + \frac{q_2}{\alpha_2} \frac{\hat{i}' + \hat{j}'}{\sqrt{2}} + \frac{q_3}{\alpha_2} \frac{-\hat{i}' + \hat{j}' + 2\hat{k}'}{\sqrt{6}} \right.$$

$$\left. + \frac{q_4}{\alpha_3} \frac{-\hat{j}' + \hat{k}'}{\sqrt{2}} + \frac{q_5}{\alpha_3} \frac{-\hat{i}' - \hat{k}'}{\sqrt{2}} + \frac{q_6}{\alpha_3} \frac{\hat{i}' - \hat{j}'}{\sqrt{2}} \right\}$$

$$\vec{r}_3 = a \left\{ \left(1 + \frac{q_1}{\alpha_1}\right) \frac{-\hat{i}' - \hat{j}' + \hat{k}'}{\sqrt{3}} + \frac{q_2}{\alpha_2} \frac{\hat{i}' - \hat{j}'}{\sqrt{2}} + \frac{q_3}{\alpha_2} \frac{-\hat{i}' - \hat{j}' - 2\hat{k}'}{\sqrt{6}} \right.$$

$$\left. + \frac{q_4}{\alpha_3} \frac{\hat{j}' - \hat{k}'}{\sqrt{2}} + \frac{q_5}{\alpha_3} \frac{\hat{i}' - \hat{k}'}{\sqrt{2}} + \frac{q_6}{\alpha_3} \frac{-\hat{i}' - \hat{j}'}{\sqrt{2}} \right\}$$

$$\vec{r}_4 = a \left\{ \left(1 + \frac{q_1}{\alpha_1}\right) \frac{\hat{i}' + \hat{j}' + \hat{k}'}{\sqrt{3}} + \frac{q_2}{\alpha_2} \frac{-\hat{i}' + \hat{j}'}{\sqrt{2}} + \frac{q_3}{\alpha_2} \frac{\hat{i}' + \hat{j}' - 2\hat{k}'}{\sqrt{6}} \right.$$

$$\left. + \frac{q_4}{\alpha_3} \frac{\hat{j}' + \hat{k}'}{\sqrt{2}} + \frac{q_5}{\alpha_3} \frac{\hat{i}' + \hat{k}'}{\sqrt{2}} + \frac{q_6}{\alpha_3} \frac{\hat{i}' + \hat{j}'}{\sqrt{2}} \right\}$$

in which

a is a characteristic distance, the "nuclear radius" appropriate to the model, the radius of the configuration with all $q_i = 0$.

$\alpha_1, \alpha_2, \alpha_3$ are numbers ~ 3 associated with the three types of vibration.

Values which are consistent with the model are:

$$a = \left(\frac{9}{4} \quad \frac{h^2}{MW_3}\right)^{1/2} = 1.9 \times 10^{-13} \text{ cm} \qquad (M = \alpha\text{-particle mass})$$

$$\alpha_1 = \left(\frac{4Ma^2 w_1}{\hbar}\right)^{1/2} = 3 \left(\frac{w_1}{W_3}\right)^{1/2} = 2.98$$

$$\alpha_2 = 3 \left(\frac{w_2}{W_3}\right)^{1/2} \begin{array}{l} = 2.40 \text{ on identification (b)} \\ = 3.15 \text{ on identification (a)} \end{array}$$

$$\alpha_3 = 3 \left(\frac{w_3}{W_3}\right)^{1/2} \begin{array}{l} = 2.66 \text{ on identification (b)} \\ = 2.63 \text{ on identification (a).} \end{array}$$

2.1. Normalized Wave Functions.

$(0,0,0,0^+)$ Ground state

$$\Psi_o = (8\pi^2)^{-1/2} \pi^{-3} \exp(-\frac{1}{2} \sum_{i=1}^{6} q_i^2)$$

$(1,0,0,0^+)$ Excitation Energy $W_o = w_1 = 6.06$ Mev

$$\Psi_{o'} = \sqrt{2}\, q_1 \Psi_o .$$

$(0,0,0,3^-)$ Excitation Energy $W_3 = 6w_o = 6.14$ Mev

$$W_{3-}^{m} = \sqrt{7} \frac{1}{\sqrt{2}} [Y_{3-}^{2,m}(\Gamma) - Y_{3-}^{-2,m}(\Gamma)] \Psi_o .$$

$(0,2,0,2^+)$ Excitation Energy $W_2 = w_2 + 3w_o = 6.91$ Mev on identification (b)

$$\Psi^m_{2+} = \sqrt{5}\ \sqrt{2}\ \frac{1}{2} \left\{ \sqrt{2}\ q_3\ Y^{o,m}_{2+}(\Gamma) + q_2[Y^{2,m}_{2+}(\Gamma) + Y^{-2,m}_{2+}(\Gamma)] \right\} \Psi_o \ .$$

$(0,0,1,2^+)$ Excitation Energy $W_1' = w_3 + 9w_o/4 = 7.01$ Mev on identification (a).

$$\Psi^m_{2'+} = \sqrt{5}\ \sqrt{2}\ \frac{1}{\sqrt{6}} \left\{ \sqrt{2}\ v_1^1\ Y^{-1,m}_{2+}(\Gamma) + v_1^o\ [Y^{2,m}_{2+}(\Gamma) - Y^{-2,m}_{2+}(\Gamma)] - \sqrt{2}\ v_1^{-1}\ Y^{1,m}_{2+}(\Gamma) \right\} \Psi_o \ .$$

$(0,0,1,1^-)$ Excitation Energy $W_1 = w_3 + 9w_o/4 = 7.21$ Mev on identification (b).

$$\Psi^m_{1-} = \sqrt{3}\ \sqrt{2}\ \frac{1}{\sqrt{3}} \left\{ v_1^1\ Y^{1,m}_{1-}(\Gamma) + v_1^o\ Y^{o,m}_1(\Gamma) + v_1^{-1}\ Y_1^{-1,m}(\Gamma) \right\} \Psi_o \ .$$

In the above

$$v_1^1 = -\frac{1}{\sqrt{2}}(q_4 + iq_5)$$

$$v_1^o = q_6$$

$$v_1^{-1} = \frac{1}{\sqrt{2}}(q_4 - iq_5) \ .$$

2.2. A Note on Matrix Elements.

In computing a matrix element

$$\langle a|0|b\rangle = (\Psi_a, 0\Psi_b) = \int \Psi_a^* \, 0\Psi_b \, d\tau \ ,$$

the volume element we employ is

$$d\tau = dq_1, dq_2, \ldots , dq_6 \sin\theta \, d\Psi \, d\phi \, d\theta$$

with $0 < \Psi, \phi < 2\pi$; $-\infty < q_i < \infty$ as limits of integration, and with the operator O expressed in terms of q_i and $\Gamma(\phi, \theta, \Psi)$. The wave functions are normalized and orthogonalized accordingly.

This procedure corresponds to the use of the barred momenta, wave functions and Hamiltonian of sec. I.2.2.2.

[It can be argued that the limits $-\infty < q_i < \infty$ are not mathematically true to the model, inasmuch as the assumed potentials certainly break down as $|q_i/\alpha_i| \to 1$, and cannot apply for $|q_i| > \alpha_i$. Further, the condition of sec. I.2.1 on the Jacobian of the transformation has been violated by the time $q_1 = -\alpha_1$, for example. This situation is not serious, however, since all α_i are ≥ 2.4 and since $e^{-\alpha_i^2} < .003$, the errors that arise from this cause will be only a few per cent.]

2.3. Expression of Operators.

Any operators used will have to be expressed in terms of the coordinates $q_1, \ldots, q_6, \Gamma$. The operators will appear in terms of the radial and angular coordinates* associated with each of the particles; however, by virtue of the wave function symmetry, we may choose a particular particle, say number 4, in terms of which to perform all calculations.

Thus we shall require expressions for r_4, Γ_4 in terms of q_i and Γ. When we compute the matrix elements between any singly-

---

* There also could occur the angular momentum of a particle, as for example in expression of magnetic multipole operators. However none of our calculations will require an expression for $\vec{J}_4$.

excited vibrational state and the ground, it will suffice to use a first order expansion in the q_i. However in a later calculation of the quadrupole moment of the ground state of O^{17}, a second order expansion is required.

(1) <u>The Operator</u> r_4.

To first order:

$$r_4 = a \left\{ 1 + \frac{q_1}{\alpha_1} + \frac{2}{\sqrt{6}} \, \frac{1}{\alpha_3} (q_4 + q_5 + q_6) \right\}.$$

To second order:

$$\begin{aligned}(r_4)^2 = a^2 \Big\{ & 1 + \left(\frac{q_1}{\alpha_1}\right)^2 + \frac{1}{\alpha_2^2} (q_2^2 + q_3^2) + \frac{1}{\alpha_3^2} (q_4 + q_5 + q_6)^2 \\ & + \frac{4}{\sqrt{6}} \left[1 + \frac{q_1}{\alpha_1} \right] \left[\frac{1}{\alpha_3} (q_4 + q_5 + q_6) \right] + \\ & + \frac{1}{\sqrt{3} \, \alpha_2 \alpha_3} (\sqrt{3} \, q_2 [q_4 - q_5] + q_3 [2q_6 - q_4 - q_5]) \\ & - \frac{1}{\alpha_3^2} (q_4 q_5 + q_5 q_6 + q_4 q_6) \Big\} .\end{aligned}$$

(2) <u>The Operator</u> Γ_4.

We can obtain the rotation Γ_4 by a three step process. By definition, Γ_4 is the rotation necessary to take a set of axes $\hat{i}'''$, $\hat{j}'''$, $\hat{k}'''$ such that $\vec{r}_4$ lies on $\hat{k}'''$ and turn them into the fixed $\hat{i}, \hat{j}, \hat{k}$ axes. We can break this up into: first a rotation Γ_q which brings $\hat{i}'''$, $\hat{j}'''$, $\hat{k}'''$ into $\hat{i}''$, $\hat{j}''$, $\hat{k}''$ in which $\hat{k}''$ is the axis on which "4" would lie of all $q_i = 0$; second a rotation Γ_4' which brings $\hat{i}''$, $\hat{j}''$, $\hat{k}''$ into $\hat{i}'$, $\hat{j}'$, $\hat{k}'$; third the rotation Γ which brings $\hat{i}'$, $\hat{j}'$, $\hat{k}'$ into $\hat{i}$, $\hat{j}$, $\hat{k}$.

Thus: $\Gamma_4 = \Gamma_q \Gamma_4' \Gamma$.

(Alternatively, the rotation Γ_4^{-1} which carries the vector $a\hat{k}$ into the vector $r_4\hat{k}'''$ is made up of Γ^{-1} which carries $a\hat{k}$ into $a\hat{k}'$, followed by $\Gamma_4'^{-1}$ which carries $a\hat{k}'$ into $a\hat{k}'' = a(\frac{\hat{i}' + \hat{j}' + \hat{k}'}{\sqrt{3}})$, followed by Γ_q^{-1} which carries $a\hat{k}''$ into $r_4\hat{k}'''$: $\Gamma_4^{-1} = \Gamma^{-1} \Gamma_4'^{-1} \Gamma_4^{-1}$ or again $\Gamma_4 = \Gamma_q \Gamma_4' \Gamma$.)

We choose $\hat{i}'' = \frac{-\hat{i}' - \hat{j}' + 2\hat{k}'}{\sqrt{6}}$; $\hat{j}'' = \frac{\hat{i}' - \hat{j}'}{\sqrt{2}}$; $\hat{k}'' = \frac{\hat{i}' + \hat{j}' + \hat{k}'}{\sqrt{3}}$.

Then the rotation Γ_4' is given by $(\phi, \theta, \Psi) = (0, \sin^{-1}\sqrt{\frac{2}{3}}, \frac{3}{4}\pi)$.

Γ_q is obtained by noting that

$$\vec{r}_4 \cdot \hat{i}'' = a\left\{\frac{-q_3}{a_2} + \frac{q_4 + q_5 - 2q_6}{2\sqrt{3}\, a_3}\right\}$$

$$\vec{r}_4 \cdot \hat{j}'' = a\left\{\frac{-q_2}{a_2} - \frac{q_4 - q_5}{2a_3}\right\}$$

$$\vec{r}_4 \cdot \hat{k}'' = a\left\{1 + \frac{q_1}{a_1} + \frac{2}{\sqrt{6}\, a_3}[q_4 + q_5 + q_6]\right\} .$$

Since a rotation about $\hat{i}''$ carries $\hat{k}''$ into $-\hat{j}''$, while a rotation about $\hat{j}''$ carries $\hat{k}''$ into $\hat{i}''$, the required notation is $\frac{-q_2}{a_2} - \frac{q_4 - q_5}{2a_3}$ about $\hat{i}''$ plus $\frac{q_3}{a_2} + \frac{2q_6 - q_4 - q_5}{2\sqrt{3}\, a_3}$ about $\hat{j}''$, or since an infinitesimal rotation about $\hat{i}''$ or $\hat{j}''$ is brought about by the operator iS_x' or iS_y' respectively, then to first order, Γ_q is represented by the operator

$$\Gamma_q = 1 - i\left\{\frac{q_2}{a_2} + \frac{q_4 - q_5}{2a_3}\right\} S_x' + i\left\{\frac{q_3}{a_2} + \frac{2q_6 - q_4 - q_5}{2\sqrt{3}\, a_3}\right\} S_y' .$$

If we need the Γ_q operator to second order in q_i, we regard the rotation Γ_q as a finite rotation through θ''_x about i" and through θ''_y about j". (Any physically important operators will be represented by terms $Y^{o,m}_{J\pm}(r_4)$. Thus any S'_z term in Γ_q will yield nothing and it does not matter whether θ''_x precedes θ''_y, θ''_y precedes θ''_x or the two rotations are simultaneous, since $S'_x S'_y - S'_y S'_x = \frac{i}{2} S'_z$.) We then use a second order expansion in θ''_x and θ''_y and keep terms of second order in q_i, obtaining:

$$
\begin{aligned}
\Gamma_q = 1 &- \frac{\sqrt{6}}{2} \frac{q_1}{\alpha_1 \alpha_3} (q_4 + q_5 + q_6) - \frac{1}{6\alpha_3^2} (q_4 + q_5 + q_6)^2 \\
&+ \frac{1}{2\alpha_3^2} (q_4 q_5 + q_5 q_6 + q_4 q_6) - \frac{1}{2\alpha_2^2} (q_2^2 + q_3^2) \\
&- \frac{\sqrt{3}}{6\alpha_2\alpha_3} \left(\sqrt{3}\, q_2[q_4 - q_5] + q_3[2q_6 - q_4 - q_5] \right) \\
&+ \left(1 - \frac{q_1}{\alpha_1} - \frac{2}{\alpha_3\sqrt{6}} [q_4 + q_5 + q_6] \right) \left(-i \left[\frac{q_2}{\alpha_2} + \frac{q_4 - q_5}{2\alpha_3} \right] S'_x \right. \\
&\qquad\qquad \left. + i \left[\frac{q_3}{\alpha_2} + \frac{2q_6 - q_4 - q_5}{2\alpha_3\sqrt{3}} \right] S'_y \right) \\
&- \frac{1}{2} \left(\frac{q_2}{\alpha_2} + \frac{q_4 - q_5}{2\alpha_3} \right)^2 (S'_x)^2 - \frac{1}{2} \left(\frac{q_3}{\alpha_2} + \frac{2q_6 - q_4 - q_5}{2\alpha_3\sqrt{3}} \right)^2 (S'_y)^2 \\
&+ \frac{1}{2} \left(\frac{q_2}{\alpha_2} + \frac{q_4 - q_5}{2\alpha_3} \right) \left(\frac{q_3}{\alpha_2} + \frac{2q_6 - q_4 - q_5}{2\alpha_3\sqrt{3}} \right) (S'_x S'_y + S'_y S'_x) + \cdots .
\end{aligned}
$$

3.0. Emission of Quanta.

In the α-model of 0^{16} the α-particles may be treated non-relativistically. Thus to perform the lifetime calculations for all except the 0^+ state, we start with the non-relativistic Hamiltonian for a set of particles of mass M, charge Ze (Z = 2 here; for an electron Z would be −1), and spin zero in an electromagnetic field with vector potential $\vec{A}$ and scalar potential .

$$H = \sum_{i=1}^{4} \frac{1}{2M} (\vec{p}_i - \frac{Ze}{c} \vec{A}(\vec{r}_i))^2 + V(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) + \sum_{i=1}^{4} Ze\, \Phi (r_i)$$

$$= H_o + \mathcal{H}_1 + \mathcal{H}_2 \quad \text{, where}$$

$H_o = \frac{1}{2M} \sum_{i=1}^{4} (\vec{p}_i)^2 + V(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4)$ is our original zero-order Hamiltonian for the α-particle model, and

$$\mathcal{H}_1 = \frac{-Ze}{2Mc} \sum_{i=1}^{4} (\vec{p}_i \cdot \vec{A}(\vec{r}_i) + \vec{A}(\vec{r}_i) \cdot \vec{p}_i) + Ze \sum_{i=1}^{4} \Phi (\vec{r}_i)$$

$$\mathcal{H}_2 = \frac{Z^2 e^2}{2Mc^2} \sum_{i=1}^{4} A^2(r_i)$$

are perturbation Hamiltonians corresponding to the emitted electromagnetic radiation.

According to the rules of Quantum Electrodynamics:

1. We can choose the gauge such that $\Phi = 0$.
2. An emitted photon of energy E, momentum $\vec{K}$ $(K = \frac{E}{c})$ and polarization $\vec{e}$ is represented by the vector potential:

$$\vec{A} = (4\pi\hbar^2 c^2)^{1/2} \vec{e}\, e^{\frac{i}{\hbar} (Et - \vec{K}\cdot\vec{x})} \quad ; \quad \vec{e} \cdot \vec{K} = 0.$$

The normalization used here is the relativistic normalization in which a plane wave, representing a particle of energy E, is normalized to a probability of finding 2E photons per cubic centimeter.

3. The probability of emission of a photon is to be calculated by perturbation theory, but the vector potential for a single photon acts only once in the perturbation. Thus the $\mathcal{H}_2$ term can emit or absorb two photons or emit one and absorb the other, but can never figure in a single photon emission process.

The transition rate ω from a state 1 to a state 0 through the action of a perturbation Hamiltonian $\mathcal{H}$ is given by

$$\omega = \frac{2\pi}{\hbar N} \mathcal{S} \, |\mathcal{H}_{01}|^2 \rho$$

where ρ is the density of final states,

$\mathcal{H}_{01}$ is the matrix element of $\mathcal{H} = \int \Psi_0^* \mathcal{H} \Psi_1 d\tau = <0|\mathcal{H}|1>$

$\mathcal{S}$ denotes an average over initial states and a sum over final states.

N is a normalizing factor: in our method of normalization N is the product of a factor $2E_i$ for every free particle of energy E_i in the final state.

3.1. Single Photon Emission.

For the particular case of state 1 with energy W_1, spin J_1 and z component of spin m_1, going into state 0 with energy W_o, spin J_o, z component m_o, with emission of a photon of energy $E = W_1 - W_o$ into solid angle $d\,\Omega$.

$$\rho = \frac{E^2 d\Omega}{(2\pi\hbar c)^3}$$

$$\mathcal{H} = \frac{-Ze}{2Mc} (4\pi\hbar^2 c^2)^{1/2} \sum_{i=1}^{4} [(\vec{e}\cdot\vec{p}_i)\, e^{\frac{i}{\hbar}(Et-\vec{K}\cdot\vec{x}_i)} + e^{\frac{i}{\hbar}(Et-\vec{K}\cdot\vec{x}_i)} (\vec{e}\cdot\vec{p}_i)]$$

$$= \frac{-Ze}{Mc} (4\pi\hbar^2 c^2)^{1/2} \sum_{i=1}^{4} e^{\frac{i}{\hbar}(Et-\vec{K}\cdot\vec{x}_i)} (\vec{e}\cdot\vec{p}_i)$$

since $\vec{K} \cdot \vec{e} = 0$.

$$\mathcal{S} = \frac{1}{(2J_1 + 1)} \sum_{\text{polarizations}} \sum_{m_1=-J_1}^{J_1} \sum_{m_o=-J_o}^{J_o} \quad .$$

If we seek the total transition rate (assuming that this process predominates), and deal with an initially unoriented state, then the sum over polarizations yields the factor 2, and integration over $d\Omega$ yields 4π . Further, all of the wave functions we deal with are symmetric in interchange of any of the four α's, so the $\sum_{i=1}^{4}$ in $\mathcal{H}$ will yield the factor 4, and we get

$$\omega = \frac{2\pi}{\hbar} \cdot \frac{1}{2E} \cdot \frac{2}{(2J_1 + 1)} \cdot \frac{4\pi E^2}{(2\pi\hbar c)^3} \cdot 4\pi\hbar^2 c^2 \cdot (4Ze)^2\, \mathfrak{M}$$

and putting $Z = 2$

$$\omega = \frac{2^8}{2J_1 + 1} \left(\frac{e^2}{\hbar c}\right) \frac{E}{\hbar}\, \mathfrak{M}$$

and

$$\mathfrak{M} = \sum_{m_1=-J_1}^{J_1} \sum_{m_o=-J_o}^{J_o} \left| <0,m_o \left| \frac{e\cdot p_i}{Mc}\, e^{\frac{i}{\hbar}(Et-\vec{K}\cdot\vec{r}_i)} \right| 1,m_1> \right|^2 \quad .$$

The mean life τ of the state is then given by

$$\tau = \frac{1}{\omega} \ .$$

3.2. Multipole Expansion.

In the calculations of the matrix element sums M, we can choose any $i = 1, 2, 3, 4$ (any other choice would be equivalent) and choose photons in the +z direction $\vec{K} = \frac{E}{c}\hat{k}$ with polarization in the x-direction $\vec{e} = \hat{i}$.

We need the matrix elements of the operator

$$\frac{\vec{e}\cdot\vec{p}_i}{Mc}\, e^{\frac{c}{\hbar}(\vec{K}\cdot\vec{r}_i)} .$$

However instead of using this operator directly in computing matrix elements, we use a multipole expansion, based on the fact that the exponential is expressible as a power series in $\frac{\vec{K}\cdot\vec{r}}{\hbar}$ which is of order $\frac{Ea}{\hbar c}$ and that for any particular wave functions the non-vanishing terms differ in order of magnitude by the square of this quantity

$$\left(\frac{Ea}{\hbar c}\right)^2 = \left(\frac{E}{2m_oc^2}\right)^2 \quad \left(\frac{a}{a_o}\right)^2$$

where m_o = mass of electron and a_o = Bohr radius = $\frac{\hbar}{2m_oc}$. $\frac{E}{2m_oc^2} \sim 6$ and $\frac{a}{a_o} \sim \frac{3}{2000} = 1.5 \times 10^{-3}$, so that the successive non-vanishing contributions differ in magnitude by a factor 10^{-4}.

We shall require the expansion to third order (second order in $\frac{\vec{K}\cdot\vec{r}}{\hbar}$),

$$\frac{\vec{e}\cdot\vec{p}}{Mc}\, e^{\frac{i}{\hbar}(\vec{K}-\vec{r})} = \frac{\vec{e}\cdot\vec{p}}{Mc}\left(1 + \frac{i}{\hbar}\,\vec{K}\cdot\vec{r} - \frac{1}{2\hbar^2}\,(\vec{K}\cdot\vec{r})^2 + \cdots\right) .$$

(1) First order terms: Electric Dipole operator.

By operator calculus,

$$\frac{\vec{e}\cdot\vec{p}}{Mc} = \frac{d}{dt}\,\frac{\vec{e}\cdot\vec{r}}{c} = \frac{iE}{\hbar c}\,\vec{e}\cdot\vec{r} .$$

Putting $\vec{e} = \hat{i}$, we get

$$\frac{iE}{\hbar c} x \quad .$$

(2) <u>Second order terms</u>:

Put $\vec{K} = \frac{E}{e}\hat{k}$

$$\frac{i(\vec{e}\cdot\vec{p})(\vec{K}\cdot\vec{r})}{M\hbar c} = \frac{E}{2}\left[\frac{(\vec{e}\cdot\vec{p})(\hat{k}\cdot\vec{r}) + (\vec{e}\cdot\vec{r})(\hat{k}\cdot\vec{p})}{M\hbar c}\right]$$

$$+ \frac{E}{2}\left[\frac{(\vec{e}\cdot\vec{p})(\hat{k}\cdot\vec{r}) - (\vec{e}\cdot\vec{r})(\hat{k}\cdot\vec{p})}{M\hbar c}\right]$$

From the first of these terms arises the electric quadrupole operator

$$\frac{iE}{\hbar c}\,\frac{d}{dt}\,[(\vec{e}\cdot\vec{r})(\hat{k}\cdot\vec{r})] = \frac{-E^2}{2\hbar^2 c}(\vec{e}\cdot\vec{r})(\hat{k}\cdot\vec{r})$$

$$= \frac{-E^2}{2\hbar^2 c^2}\; zx \; .$$

From the second arises the magnetic dipole operator

$$\frac{E}{2\hbar Mc^2}(\vec{r} \times \vec{p}) \cdot \hat{j} \; .$$

(3) <u>Third order terms</u>:

$$\frac{-(\vec{e}\cdot\vec{p})(\vec{K}\cdot\vec{r})^2}{2M\hbar^2 c} = \frac{-E^2}{2M\hbar^2 c^3}(\vec{e}\cdot\vec{p})(\hat{k}\cdot\vec{r})^2$$

$$= \frac{-E^2}{\hbar^2 c^3}\;\frac{1}{30}\;\frac{d}{dt}\,[(\vec{e}\cdot\vec{r})(5[\hat{k}\cdot\vec{r}]^2 - r^2]$$

$$+ \frac{1}{6M}\,[2(\vec{e}\cdot\vec{p})(k\cdot\vec{r})^2 - (\vec{e}\cdot\vec{r})[(\hat{k}\cdot\vec{p})(k\cdot\vec{r}) + (\hat{k}\cdot\vec{r})(\hat{k}\cdot\vec{p})]]$$

$$+ \frac{1}{30}\;\frac{d}{dt}\;[r^2(\vec{e}\cdot\vec{r})]$$

The first term gives rise to the Electric Octupole operator

$$\frac{-iE^3}{30\hbar^3 c^2}\,(\vec{e}\cdot\vec{r})\;(5[k\cdot\vec{r}]^2 - r^2) = \frac{-iE^3}{30\hbar^3 c^3}\;x(5z^2 - r^2)\ .$$

The second term is the Magnetic Quadrupole operator:

$$\frac{-E^2}{6M\hbar^2 c^3}\,[\,\hat{j}\cdot(\vec{r}\times\vec{p})\,z + z(\vec{r}\times\vec{p})\cdot\hat{j}\,]\ .$$

The third term is a third order Electric Dipole operator:

$$\frac{-iE^3}{30\hbar^3 c^3}\;r^2(\vec{e}\cdot\vec{r}) = \frac{-iE^3}{30\hbar^3 c^3}\,r^2 x\ .$$

3.2.1. Electric Multipole Operators.

In the calculations, we need expressions for the electric multipole operators in terms of radial coordinate r_4 and angular coordinates Γ_4. In this we regard r_4 as invariant under permutation. Thus the parity of the angular functions for an electric multipole of order l is $(-1)^l$.

The electric multipole operators $\mathcal{E}_l$ are:

(1) Electric Dipole:

$$\mathcal{E}_1 = \frac{iE}{\hbar c}\,\frac{r_4}{\sqrt{2}}\,(Y^{0,-1}_{1-}(\Gamma) - Y^{0,1}_{1}(\Gamma_4)) \quad \text{(first order)}$$

$$\mathcal{E}^{(3)}_1 = \frac{-iE^3}{\hbar^3 c^3}\;\frac{r_4^3}{30\sqrt{2}}\,(Y^{0,-1}_{1-}(\Gamma_4) - Y^{0,1}_{1-}(\Gamma_4)) \quad \text{(third order).}$$

Either of these operators can induce $\Delta J = 0, 1;\ \Delta m = 1$, parity change transitions (no 0 → 0). Normally $\mathcal{E}_1$ would be two orders of magnitude larger than $\mathcal{E}^{(3)}_1$ except that in the case N identical particles, the matrix element of $\vec{r}_i$ is just $\frac{1}{N}$ x the matrix element of $\vec{X}$, and since $\vec{X} = 0$, the matrix element of $\mathcal{E}_1$ always vanishes, and only $\mathcal{E}_1^{(3)}$ can contribute.

(2) Electric Quadrupole:

$$\mathcal{E}_2 = \frac{-E^2}{\hbar^2 c^2} \frac{r_4^2}{\sqrt{24}} (Y_{2+}^{o,-1}(\Gamma_4) - Y_{2+}^{o,1}(\Gamma_4)) \ .$$

This operator can induce $\Delta J = 0, 1, 2$; $\Delta m = 1$, no parity change (no $0 \to 0$, $1 \to 0$, $0 \to 1$) transitions.

(3) Electric Octupole:

$$\mathcal{E}_3 = \frac{-iE^3}{\hbar^3 c^3} \frac{r_4^3}{15\sqrt{3}} (Y_{3-}^{o,-1}(\Gamma_4) - Y_{3-}^{o,1}(\Gamma_4)) \ .$$

This operator can induce $\Delta J = 0, 1, 2, 3$; $\Delta m = 1$, parity change (no $0, 1 \to 0, 1$; $2 \to 0$; $0 \to 2$) transitions.

3.2.2. Magnetic Multipole Operators.

In our calculations, we shall never employ the magnetic multipole operators. In general a magnetic 2^l pole has parity $(-1)^{l-1}$ and carries angular momentum $l\hbar$, except that for a set of identical Bose particles, the magnetic dipole operator can never change the total angular momentum.

(1) Magnetic Dipole:

$$\mathcal{M}_1 = \frac{e}{2Mc^2} \frac{1}{\hbar} (\vec{r}_4 \times \vec{p}_4) \cdot \hat{j} \ .$$

The total angular momentum, $\hbar \vec{J} = \sum_i (\vec{r}_i \times \vec{p}_i)$ where the sum is over all particles. In any matrix element of $\vec{J}$ for identical

Bose particles, however, each particle contributes equally by virtue of the symmetry of wave functions and thus for N particles, we can replace

$$\frac{1}{\hbar}(\vec{r}_i \times \vec{p}_i) = \frac{1}{N}\vec{J}\,, \qquad \text{or in our case}$$

$$= \frac{e}{8Mc^2}\vec{J}\cdot\hat{j} = \frac{ie}{16Mc^2}(S_- - S_+)\,.$$

Thus in this model, the magnetic dipole operator can induce only transitions in which $\Delta J = 0$, $\Delta m = \pm 1$, no parity change.

(2) Magnetic Quadrupole.

$$\mathcal{M}_2 = \frac{-E^2}{6Mc^3\hbar^3}[\hat{j}\cdot(\vec{r}_4 \times \vec{p}_4)z_4 + z_5(\vec{r}_4 \times \vec{p}_4)\cdot\hat{j}\,]$$

$$= \frac{-E^2}{6Mc^3\hbar^3}[\hat{j}\cdot\vec{J}_4\, z_4 + z_4\,\vec{J}_4\cdot\hat{j}\,]\,.$$

An expression for $\vec{J}_4$ can be found but the procedure is messy and has not been carried out. The form of the expression which would be obtained for $\mathcal{M}_2$ is

$$\mathcal{M}_2 = \frac{-E^2\ a}{6Mc^3\hbar^3} f(q_i, \frac{p_i}{\hbar}, \vec{S}')\,[Y_{2-}^{0,1}(\Gamma_4) + Y_{2-}^{0,-1}(\Gamma)]\quad .$$

This operator can induce $\Delta J = 0, 1, 2$, $\Delta m = \pm 1$, parity change (no $0 \to 0$, $1 \to 0$, $0 \to 1$) transitions.

3.2.3. Transition Rates.

Finally, observing that the matrix element of the term $Y_{J,p}^{0,\mp 1}(\Gamma_i)$ between a state $\Psi_{J'p}^{m'}$ and the 0,0 ground state must vanish unless $J = J'$, $p = p'$, $m' = \pm 1$, and that magnitudes of the matrix element for $m = \pm 1$ must be equal, we have the rates:

3^- to ground

$$\omega_{30} = \frac{2^9}{7} \left(\frac{e^2}{\hbar c}\right) \frac{W_3}{\hbar} |<0,0| \mathcal{E}_3 |3^-,1>|^2 \quad .$$

2+ to ground

$$\omega_{20} = \frac{2^9}{5} \left(\frac{e^2}{\hbar c}\right) \frac{W_2}{\hbar} |<0,0| \mathcal{E}_2 |2^+,1>|^2$$

(two cases to consider, according to the identification used).

1^- to ground. In first order

$$\omega_{10} = \frac{2^9}{3} \left(\frac{e^2}{\hbar c}\right) \frac{W_1}{\hbar} \; |<0,0| \mathcal{E}_1 |1^-,1>|^2$$

which vanishes, and we are left with

$$\omega_{10}^{(3)} = \frac{2^9}{3} \left(\frac{e^2}{\hbar c}\right) \frac{W_1}{\hbar} \; |<0,0| \mathcal{E}_1^{(3)} |1^-,1>|^2 \quad .$$

3.3. Calculation of Matrix Elements.

(1) $3^- \rightarrow 0$

$$B_3 = <0,0| \mathcal{E}_3 |3^-,1> \quad .$$

$$\Psi_3^1 = \sqrt{7} \, \frac{1}{\sqrt{2}} \, [Y_{3-}^{2,m}(\Gamma) - Y_{3-}^{-2,m}(\Gamma)] \, \Psi_o \quad .$$

$$\mathcal{E}_3(\vec{r}_4) = \frac{-i}{15\sqrt{3}} \left(\frac{W_3 r_4}{\hbar c}\right)^3 \, Y_{3-}^{o,-1}(\Gamma_4) \quad .$$

We need the zeroth order expansion of r_4 and Γ_4 in terms of q_i:

$$r_4 = a$$

$$\Gamma_4 = \Gamma_q \, \Gamma_4' \, \Gamma \qquad \text{with} \qquad \Gamma_q = 1 \quad .$$

Whence

$$Y_{3-}^{o,-1}(\Gamma_4) = \sum_{h=-3}^{3} Y_{3-}^{o,h}(\Gamma_4') \, Y_{3-}^{h,-1}(\Gamma)$$

and the only terms which can survive integration over Ψ are those with $h = \pm 2$.

$$\Gamma'_4 \equiv (0, \sin^{-1}\sqrt{\tfrac{2}{3}}, \tfrac{3}{4}\pi)$$

$$Y^{0,\pm2}_{3-}(\Gamma'_4) = e^{\pm3i\pi/2}\, P^{0,\pm2}_{3-}(\sin^{-1}\sqrt{\tfrac{2}{3}}) = \mp i \frac{\sqrt{30}}{4} \cdot \frac{2}{3}\sqrt{\frac{1}{3}}$$
$$= \mp i \frac{\sqrt{10}}{6} ;$$

whence

$$B_3 = \left(\frac{W_3 a}{\hbar c}\right)^3 \Big(\Psi_o, \frac{\sqrt{7}}{\sqrt{2}} \cdot \frac{1}{15\sqrt{3}} \times \frac{\sqrt{10}}{6} [Y^{-2,-1}_{3-}(\Gamma) - Y^{2,-1}_{3-}(\Gamma)]$$
$$[Y^{2,1}_{3-}(\Gamma) - Y^{-2,1}_{3-}(\Gamma)]\, \Psi_o\Big) .$$

Now $Y^{\mp2,-1}_{3-} = -(Y_3^{\pm2,-1})^*$ and the only terms which can survive the integration are the products $Y^{-2,-1}_{3-}\, Y^{2,1}_{3-}$ and $Y^{2,-1}_{3-}\, Y^{-2,1}_{3-}$ which each yield $\frac{1}{7}$

$$B_3 = -\frac{1}{9\sqrt{105}} \left(\frac{W_3 a}{\hbar c}\right)^3 .$$

(2) $\underline{2^+ \to 0}$

$$B_2 = \langle 0,0|\,\xi_2\,|2^+,1\rangle$$

$$\Psi'_2 = \sqrt{5}\,\sqrt{2}\,\frac{1}{2} \left\{ \sqrt{2}\, q_3 Y^{0,1}_{2+}(\Gamma) + q_2[Y^{2,1}_{2+}(\Gamma) + Y^{-2,1}_{2+}(\Gamma)] \right\} \Psi_o$$

$$_2(\vec{r}_4) = -\left(\frac{W_2}{\hbar c}\right)^2 \frac{r_4^2}{\sqrt{24}}\, Y^{0,-1}_{2+}(\Gamma_4)$$

and we need the first order expansion of r_4 and Γ_4 in terms of q_2 and q_3:

$$r_4 = a$$

$$\Gamma_4 = \Gamma_q\, \Gamma'_4\, \Gamma \quad \text{with} \quad \Gamma_q = 1 - i\frac{q_2}{\alpha_2} S'_x + i\frac{q_3}{\alpha_2} S'_y .$$

Only the S'_x and S'_y terms can produce a finite matrix element:

$$S'_x = \frac{1}{2}\,(S'_+ + S'_-) \qquad\qquad S'_y = \frac{i}{2}\,(S'_- - S'_+)$$

$$Y_{2+}^{o,-1}(\Gamma'_4\,\Gamma) = \sum_{h=-2}^{2} Y_{2+}^{o,h}(\Gamma'_4)\; Y_{2+}^{h,-1}(\Gamma)$$

$$S'_x\, Y_{2+}^{o,h} = \frac{1}{2}\;\sqrt{6}\;(Y_{2+}^{1.h} + Y_{2+}^{-1,h})$$

$$S'_y\, Y_{2+}^{o,h} = \frac{i}{2}\;\sqrt{6}\;(Y_{2+}^{1,h} - Y_{2+}^{-1,h}) \quad .$$

Since only the q_2^2 and q_3^2 terms survive integration, we need:

$$Y_{2+}^{1,o}(\Gamma'_4) - Y_{2+}^{-1,o}(\Gamma'_4) = 2P_{2+}^{1,o}(\sin^{-1}\ \sqrt{\tfrac{2}{3}}\ ) = \frac{2}{\sqrt{3}}$$

$$i[Y_{2+}^{1,2}(\Gamma'_4) + Y_{2+}^{-1,2}(\Gamma'_4)] = i[Y_{2+}^{1,-2}(\Gamma'_4) + Y_{2+}^{-1,-2}(\Gamma'_4)]$$

$$= P_2^{1,2}(\sin^{-1}\ \overline{\tfrac{2}{3}}) + P_2^{-1,2}(\sin^{-1}\sqrt{\tfrac{2}{3}}) = -\,\frac{\sqrt{6}}{3}$$

and

$$Y_2^{o,-1} = -\,(Y_2^{o,1})^*, \qquad\qquad Y_2^{\mp 2,-1} = -\,(Y_2^{\pm 2,1})^* \; .$$

Putting all terms together and keeping only surviving terms:

$$B_2 = -\,i\;\left(\frac{W_2 a}{\hbar c}\right)^2 \frac{\sqrt{5}\ \sqrt{2}}{2\,\sqrt{24}}\;\frac{\sqrt{6}}{2}\;\frac{1}{a_2}\quad .$$

$$(\Psi_o,\ [2\,\frac{\sqrt{6}}{3}\,q_3^2\,|Y_{2+}^{o,1}(\Gamma)|^2 + \frac{\sqrt{6}}{3}\,q_2^2\left\{|Y_{2+}^{2,1}(\Gamma)|^2 + |Y_{2+}^{-2,1}(\Gamma)|^2\right\}\,]\Psi_o)\quad .$$

The q_3^2 and q_2^2 terms give equal contributions. From the angular integrations we get a factor 1/5 and from the q_2 or q_3 integration a factor 1/2.

$$B_2 = - i \left(\frac{W_2 a}{\hbar c}\right)^2 \frac{1}{a_2} \frac{\sqrt{5}\ \sqrt{2}}{2\sqrt{24}} \frac{\sqrt{6}}{2} \cdot \frac{2\sqrt{2}}{\sqrt{3}} \frac{1}{10} \cdot 2$$

$$B_2 = - \frac{i}{2\sqrt{15}} \frac{1}{a_2} \left(\frac{W_2 a}{\hbar c}\right)^2 .$$

(3) $\underline{2'^{+} \to 0}$

$$B_{2'} = \langle 0,0 | \mathcal{E}_2 | 2^{+\prime}, 1 \rangle$$

$$\Psi'_{2+'} = \sqrt{5}\ \sqrt{2} \frac{1}{\sqrt{6}} \Big\{ \sqrt{2}\, v_1^1\, Y_{2+}^{-1,1}(\Gamma) + v_1^o [Y_{2+}^{2,1}(\Gamma) - Y_{2+}^{-2,1}(\Gamma)]$$

$$- \sqrt{2}\, v_1^{-1}\, Y_{2+}^{1,1}(\Gamma) \Big\} \Psi_o$$

$$\mathcal{E}_2(\vec{r}_4) = - \left(\frac{W'_1}{\hbar c}\right)^2 \frac{r_4^2}{\sqrt{24}} Y_{2+}^{o,-1}(\Gamma_4) .$$

We need the first order expansion of r_4 and Γ_4 in terms of q_4, q_5, q_6:

$$r_4 = a \left(1 + \frac{2}{\sqrt{6}} \frac{1}{a_3} [q_4 + q_5 + q_6] \right)$$

$\Gamma_4 = \Gamma_q \Gamma'_4 \Gamma$, with

$$\Gamma_q = 1 - \frac{1}{2a_3} (q_4 - q_5) S'_x + \frac{i}{2\sqrt{3}\, a_3} (2q_6 - q_4 - q_5) S'_y .$$

In first order in q_4, q_5, q_6,

$$r^n \Gamma_q = \frac{a^2}{a_3} \left[\frac{2n}{\sqrt{6}} (q_4 + q_5 + q_6) - \frac{i}{2}(q_4 - q_5) S'_x + \frac{i}{2\sqrt{3}} (2q_6 - q_4 - q_5) S'_y \right].$$

Expressed in terms of

$$v_1^1 = - \frac{1}{\sqrt{2}} (q_4 + iq_5)$$

$$v_1^o = q_6$$

$$v_1^{-1} = \frac{1}{\sqrt{2}} (q_4 - iq_5) ,$$

$$q_4 \pm q_5 = e^{\pm 3\pi i/4} v_1^1 - e^{\mp 3\pi i/4} ;$$

$$r_4^n \Gamma_q = \frac{a^n}{\alpha_3} \left\{ e^{3\pi i/4} v_1^1 \left[\frac{2n}{\sqrt{6}} + \left(\frac{1}{4} - \frac{1}{4\sqrt{3}}\right) S'_+ + \left(\frac{1}{4} + \frac{1}{4\sqrt{3}}\right) S'_- \right]\right.$$

$$+ v_1^o \left[\frac{2n}{\sqrt{6}} + \frac{1}{2\sqrt{3}} (S'_+ - S'_-)\right]$$

$$\left. + e^{-3\pi i/4} v_1^{-1} \left[- \frac{2n}{\sqrt{6}} + \left(\frac{1}{4} + \frac{1}{4\sqrt{3}}\right) S'_+ + \left(\frac{1}{4} - \frac{1}{4\sqrt{3}}\right) S'_- \right]\right\}$$

$$S'_\pm Y_{2+}^{o,h} = \sqrt{6}\, Y_{2+}^{\mp 1,h} .$$

In the matrix element $B_{2'}$, the only coordinate combinations which can survive are $v_1^1 v_1^{-1}$ and $v_1^o v_1^o$, multiplied by $|Y_{2+}^{k,1}|^2$. Thus for the $v_1^{\pm 1}$ term of $_{2'}$, we need the coefficient of

$v_1^{\pm 1} Y_{1-}^{\mp 1,-1}(\Gamma_4)$ in $\dfrac{\alpha_3 r_4^n}{a^n} Y_{1-}^{o,-1}(\Gamma_4)$ which is

$$e^{\pm 3\pi i/4} \left\{ \pm \frac{2n}{\sqrt{6}} Y_{2+}^{o,\mp 1} (\Gamma'_4) + \left(\frac{1}{4} \mp \frac{1}{4\sqrt{3}}\right) \sqrt{6}\, Y_{2+}^{-1,\mp 1}(\Gamma'_4)\right.$$

$$\left. + \left(\frac{1}{4} \pm \frac{1}{4\sqrt{3}}\right) \sqrt{6}\, Y_{2+}^{1,\mp 1}(\Gamma'_4) \right\}$$

$$= \pm \frac{2n}{\sqrt{6}} P_2^{o,\pm 1} (\theta'_4) + \left(\frac{1}{4} \mp \frac{1}{4\sqrt{3}}\right) \sqrt{6}\, P_2^{-1,\mp 1} (\theta'_4)$$

$$+ \left(\frac{1}{4} \pm \frac{1}{4\sqrt{3}}\right) \sqrt{6}\, P_2^{1,\mp 1}(\theta'_4) .$$

We note that since $P_J^{o,1} = - P_J^{o,-1}$; $P_J^{11} = P_J^{-1,-1}$; $P_J^{-1,1} = P_J^{1,-1}$; the coefficients of the terms $|Y_{2+}^{1,1}|^2$ and $|Y_{2+}^{-1,1}|^2$ in the matrix element are of equal magnitude but opposite sign, and thus cancel.

There is left only the v_1^o term, for which we need:

$$\frac{2n}{\sqrt{6}} Y_{2+}^{o,\mp2}(\Gamma'_4) + \frac{1}{2\sqrt{3}} \sqrt{6}\,[Y_{2+}^{-1,\mp2}(\Gamma'_4) - Y_{2+}^{1,\mp2}(\Gamma'_4)]$$

$$= \pm i \left\{ \frac{2n}{\sqrt{6}} P_2^{o,\mp2}(\theta'_4) + \frac{1}{2\sqrt{3}} \sqrt{6}\,[P_2^{-1,\mp2}(\theta'_4) - P_2^{1,\mp2}(\theta'_4)] \right\}$$

$$P_2^{o,\pm2} = \frac{\sqrt{6}}{3}$$

$$P_2^{-1,\mp2}(\theta'_4) - P_2^{1,\mp2}(\theta'_4) = \frac{\sqrt{2}}{3} \ .$$

Thus the coefficient of $Y_{2+}^{\mp2,-1}(\Gamma)$ in $r_4^2\, Y_{2+}^{o,-1}(\Gamma_4)$ is

$$\pm i \frac{a^2}{a_3} \quad \frac{4}{\sqrt{6}} \cdot \frac{\sqrt{6}}{3} + \frac{\sqrt{2}}{2} \cdot \frac{\sqrt{6}}{3} \quad = \pm \frac{5}{3} i \frac{a^2}{a_3} \ .$$

From the integration of $|Y_{2+}^{\pm2,1}|^2$ we get a factor 1/5 and from the $(v_1^o)^2$ a factor 1/2, yielding:

$$B_{2'} = - \frac{W'_1 a}{\hbar c}^{2} \frac{1}{a_3} \cdot \frac{\sqrt{10}}{\sqrt{24}} \cdot \frac{1}{\sqrt{6}} \cdot \frac{1}{10} \cdot 2 \cdot \frac{5}{3} i$$

$$B_{2'} = -i \frac{\sqrt{10}}{36} \frac{1}{a_3} \left(\frac{W'_1 a}{\hbar c} \right)^2 \ .$$

(4) $\underline{1^- \rightarrow 0}$

$$B_1 = \langle 0,0|\, \mathcal{E}_1 \,|1^-,1\rangle$$

$$\Psi'_1 = \sqrt{3}\ \sqrt{2}\ \frac{1}{\sqrt{3}}\ [\, v_1^1\, Y_{1-}^{1,1}(\Gamma) + v_1^o\, Y_{1-}^{o,1}(\Gamma) + v_1^{-1}\, Y_{1-}^{-1,1}(\Gamma)\,]\ \Psi_o$$

$$\mathcal{E}_1(\vec{r}_4) = \frac{iW_1}{\hbar c} \frac{r_4}{\sqrt{2}} Y_{1-}^{o,-1}(\Gamma_4) \ .$$

B_1 should vanish. From subsection (3) above the coefficient of

$$v_1^{\pm 1}\, Y_{-1}^{\pm 1,-1}(\Gamma) \quad \text{in} \quad \frac{a_3}{a^n}\, r_4^n\, Y_{1-}^{o,-1}(\Gamma_4)$$

is:

$$\mp i \left\{ \pm \frac{2n}{\sqrt{6}}\, P_1^{o,\pm 1}(\theta_4') + \left(\frac{1}{4} \mp \frac{1}{4\sqrt{3}} \right) \sqrt{2}\, P_1^{-1,\pm 1}(\theta_4') + \left(\frac{1}{4} \pm \frac{1}{4\sqrt{3}} \right) \sqrt{2}\, P_1^{1,\pm 1}(\theta_4') \right\} .$$

In the matrix element, contributions from these terms will cancel.

The coefficient of $v_1^o\, Y_{1-}^{o,-1}(\Gamma)$ in $\frac{a_3}{a^n}\, r_4^n\, Y_{1-}^{o,-1}(\Gamma_4)$ is

$$\frac{2n}{\sqrt{6}}\, P_1^{oo}(\theta_4') + \frac{1}{2\sqrt{3}}\, \sqrt{2}\, [P_1^{-1,o}(\theta_4') - P_1^{1,o}(\theta_4')] = \frac{2}{3\sqrt{2}}\, (n - 1) .$$

Thus the matrix element B_1 for which $n = 1$ vanishes.

$$B_1^{(3)} = \langle 0,0|\, \mathcal{E}_1^{(3)}\, |1^-, 1\rangle$$

$$\mathcal{E}_1^{(3)} = - i \left(\frac{W_1}{\hbar c} \right)^3 \frac{r_4^3}{30\sqrt{2}}\, Y_{1-}^{o,-1}(\Gamma_4) \quad .$$

From the above, putting $n = 3$, and noting that $Y_1^{o,-1}\, Y_1^{o,1} = - |Y_1^{o,1}|^2$, we get

$$B_1^{(3)} = i \left(\frac{W_1 a}{\hbar c} \right)^3 \frac{1}{a_3}\, \frac{1}{30\sqrt{2}} \cdot \sqrt{2} \cdot \frac{1}{3} \cdot \frac{4}{3\sqrt{2}}$$

$$B_1^{(3)} = \frac{i}{135\sqrt{2}}\, \frac{1}{a_3} \left(\frac{W_1 a}{\hbar c} \right)^3 .$$

3.4. Lifetimes: Numerical

(1) 3-state

$$\omega_{3o} = \frac{2^9}{7} \left(\frac{e^2}{\hbar c}\right) \frac{W_3}{\hbar} |B_3|^2$$

$$= \frac{2^9}{735 \times 9^2} \left(\frac{e^2}{\hbar c}\right) \left(\frac{W_3 a}{\hbar c}\right)^6 \frac{W_3}{m_o c^2} \frac{m_o c^2}{\hbar} \quad .$$

With

$$\left(\frac{W_3 a}{\hbar c}\right)^2 = \frac{9}{4} \frac{W_3}{Mc^2}$$

$$\omega_{3o} = \frac{24}{245} \left(\frac{e^2}{\hbar c}\right) \left(\frac{W_3}{Mc^2}\right)^3 \frac{W_3}{m_o c^2} \frac{m_o c^2}{\hbar}$$

(M = α-particle mass; m_o = electron mass)

$$Mc^2 = 4 \times 931 \text{ Mev}$$

$$m_o c^2 = .511 \text{ Mev}$$

$$\frac{\hbar}{m_o c^2} = 1.285 \times 10^{-21} \text{ sec.}$$

$$\tau_{3o} = \frac{1}{\omega_{3o}} = \frac{245}{24} \times 137 \times \left(\frac{4 \times 931}{6.14}\right)^3 \left(\frac{.511}{6.14}\right) \times 1.285 \times 10^{-21} \text{sec.}$$

$$\tau_{3o} = 3.2 \times 10^{-11} \text{ sec.}$$

(2) 2^+ state -Identification (b):

$$\omega_{20} = \frac{2^9}{5} \left(\frac{e^2}{\hbar c}\right) \frac{W_2}{\hbar} |B_2|^2$$

$$= \frac{2^7}{75} \left(\frac{e^2}{\hbar c}\right) \cdot \frac{1}{\alpha_2^2} \left(\frac{W_2 a}{\hbar c}\right)^4 \frac{W_2}{m_o c^2} \frac{m_o c^2}{\hbar}$$

with

$$\left(\frac{W_2 a}{\hbar c}\right)^2 = \frac{9}{4} \quad \frac{W_2}{Mc^2} \quad \frac{W_2}{W_3}$$

$$\frac{1}{a_2^2} = \frac{1}{9} \quad \frac{W_3}{w_2}$$

$$w_2 = W_2 - \frac{1}{2} W_3 = 6.91 - 3.07 = 3.84 \text{ Mev.}$$

$$\omega_{2o} = \frac{24}{25} \left(\frac{e^2}{\hbar c}\right) \quad \frac{W_2}{W_3} \quad \frac{W_2}{w_2} \left(\frac{W_2}{Mc^2}\right)^2 \quad \frac{W_2}{m_o c^2} \quad \frac{m_o c^2}{\hbar} \quad .$$

$$\tau_{2o} = \frac{1}{\omega_{2o}} = \left(\frac{25}{24}\right) (137) \left(\frac{6.14}{6.91}\right)\left(\frac{3.84}{6.91}\right)\left(\frac{4 \times 931}{6.91}\right)^2 \left(\frac{.511}{6.91}\right) \times 1.285 \times 10^{-21} \text{sec.}$$

$$\tau_{2o} = 1.95 \times 10^{-15} \text{ sec.}$$

(3) 2^+ state - Identification (a):

$$\omega_{2'o} = \frac{2^9}{5} \left(\frac{e^2}{\hbar c}\right) \frac{W_1'}{\hbar} |B_{2'}|^2$$

$$= \frac{2^6}{5 \cdot 9^2} \quad \left(\frac{e^2}{\hbar c}\right) \cdot \quad \frac{1}{a_3^2} \quad \left(\frac{W_1' a}{\hbar c}\right)^4 \quad \frac{m_o c^2}{\hbar}$$

with

$$\left(\frac{W_1' a}{\hbar c}\right)^2 = \frac{9}{4} \quad \frac{W_1'}{Mc^2} \quad \frac{W_1'}{W_3}$$

$$\frac{1}{a_{3'}^2} = \frac{1}{9} \quad \frac{W_3}{w_3'}$$

$$w_3' = W_1' - \frac{3}{8} W_3 = 7.01 - 2.30 = 4.71 \text{ Mev.}$$

$$\omega_{2'o} = \frac{4}{45} \left(\frac{e^2}{\hbar c}\right) \quad \frac{W_1'}{W_3} \quad \frac{W_1'}{w_3} \left(\frac{W_1'}{Mc^2}\right)^2 \frac{W_1'}{m_o c^2} \quad \frac{m_o c^2}{\hbar}$$

$$\tau_{2'o} = \frac{1}{\omega_{2'o}} = (\frac{45}{4})\ (137)\ (\frac{6.14}{7.01})\ (\frac{4.71}{7.01})\ (\frac{4 \times 931}{7.01})^2\ (\frac{.511}{7.01})$$

$$\times\ 1.285 \times 10^{-21} \text{sec.}$$

$$\tau_{2'o} = 2.4 \times 10^{-14} \text{ sec.}$$

(4) 1^- state

$$\omega^{(3)}_{1o} = \frac{2^9}{3}(\frac{e^2}{\hbar c})\ \frac{W_1}{\hbar}\ |B_1^{(3)}|^2$$

$$= \frac{2^9}{3.81 \times 225 \times 2}\ (\frac{e^2}{\hbar c})\ \frac{1}{a_3^2}\ \left(\frac{W_1 a}{\hbar c}\right)^6\ \frac{W_1}{m_o c^2}\ \ \frac{m_o c^2}{\hbar}$$

with

$$\left(\frac{W_1 a}{\hbar c}\right)^2 = \frac{9}{4}\ \frac{W_1}{Mc^2}\ \ \frac{W_1}{W_3}$$

$$\frac{1}{a_3^2} = \frac{1}{9}\ \frac{W_3}{w_3}$$

$$w_3 = W_1 - \frac{3}{8} W_3 = 7.21 - 2.30 = 4.91 \text{ Mev.}$$

$$\omega^{(3)}_{1o} = \frac{12}{225}\ (\frac{e^2}{\hbar c})\ \left(\frac{W_1}{W_3}\right)^2\ \ \frac{W_1}{w_3}\ \left(\frac{W_1}{Mc^2}\right)^3\ \ \frac{W_1}{m_o c^2}\ \ \frac{m_o c^2}{\hbar}$$

$$\tau^{(3)}_{1o} = \frac{1}{\omega^{(3)}_{1o}} = (\frac{225}{12})\ (137)\ (\frac{6.14}{7.21})^2\ (\frac{4.91}{7.21})\ (\frac{4 \times 931}{7.21})^3\ (\frac{.511}{7.21})$$

$$\times\ 1.285 \times 10^{-21} \text{ sec.}$$

$$\tau^{(3)}_{1o} = 1.6 \times 10^{-11} \text{ sec.}$$

4. Further Considerations on τ_{1o} .

On the strict α-particle model, first order electric dipole matrix elements vanish and so we had to resort to the third order electric dipole operator $\mathcal{E}_1^{(3)}$ to obtain a finite lifetime for the

1^- state

$$\tau_{1o}^{(3)} = 1.6 \times 10^{-11} \text{ sec.}$$

We expect that this is much too long, since a small admixture of single particle wave function would appreciably shorten this lifetime. [For a single proton outside a N^{15} shell, the transition rate would be

$$\omega_{sp} = \frac{2^5}{3} \left(\frac{e^2}{\hbar c}\right) \frac{W_1}{\hbar} \left(\frac{W_1}{\hbar c}\right)^2 < r >_{av}^2 < \sin^2 \theta >_{av} \frac{1}{2} \cdot \frac{1}{3} \ .$$

The last two factors coming from the normalization of wave functions, and with

$$< \sin^2 \theta >_{av} = \frac{2}{3} \ ;$$

$$< r >_{av}^2 = [(\tfrac{15}{16})^2 + (\tfrac{7}{16})^2] \cdot (1.3 \times 16^{1/3} \times 10^{-13} \text{ cm})^2$$

$$= \frac{274}{256} \times 1.69 \times 6.35 \times 10^{-26} \text{ cm}^2 = 1.15 \times 10^{-25} \text{ cm}^2 \ ;$$

$$\frac{\hbar}{m_o c^2} = 3.86 \times 10^{-11} \text{ cm} \ ,$$

we obtain

$$\omega_{sp} = \frac{32}{27} \frac{e^2}{\hbar c} \cdot \left(\frac{W_1}{m_o c^2}\right)^3 \cdot \frac{(1.15 \times 10^{-25})}{(3.86 \times 10^{-11})^2} \cdot \frac{m_o c^2}{\hbar}$$

$$\tau_{sp} = (\tfrac{27}{32}) \ (137) \ (\tfrac{.511}{7.21})^3 \ (\tfrac{149}{115}) \times 10^3 \times 1.28 \times 10^{-21} \text{ sec}$$

$$= 7 \times 10^{-19} \text{sec.}]$$

However, following the arguments of Wilkinson [12] we will be able to bracket the lifetime more closely.

To obtain an upper limit for the lifetime of the 1^- state we note that the 1^- state can decay to the 3^- state by electric quadrupole emission, for which our method of calculation should be valid.

Experimentally the $1^- \rightarrow 3^-$ process is observed to be less probable by a factor < .008 than the decay to ground. Hence we can obtain the upper limit $\tau_{1o} < (.008)^{-1}\, \tau_{13}$.

To obtain a lower limit we can use the fact that while the 2^+ state can decay to the 3^- state by electric dipole emission, the $2^+ \rightarrow 3^-$ process is less probable by a factor of < .005 than the $2^+ \rightarrow$ ground state decay. From $\omega_{23} < .005 \quad \omega_{2o}$ and from our previously calculated values of τ_{2o}, we can obtain an upper limit for an electric dipole matrix element. By relating the τ_{1o} to τ_{23} we can obtain a rough lower limit for τ_{1o}.

(1) <u>$1^- \rightarrow 3^-$</u>

Again we shall use only that part of $\mathcal{E}_2$ which lowers $m = J_z$.

$$B_4^m = < 3^-, m-1 |\, \mathcal{E}_2 \,| 1^-, m > \qquad \text{with} \qquad m = -1,\ 0,\ 1$$

$$\Psi_{3-}^{m-1} = \sqrt{7}\, \frac{1}{\sqrt{2}} \left[Y_{3-}^{2,m-1}(\Gamma) - Y_{3-}^{-2,m-1}(\Gamma) \right] \Psi_o$$

$$\Psi_{1-}^{o} = \sqrt{3} \;\; \sqrt{2}\, \frac{1}{\sqrt{3}} \left[v_1^1\, Y_{1-}^{1,m}(\Gamma) + v_1^o\, v_{1-}^{o,m}(\Gamma) + v_1^{-1}\, Y_{1-}^{-1,m}(\Gamma) \right] \Psi_o$$

$$\mathcal{E}_2(\vec{r}_4) = - \left(\frac{W_{13}}{\hbar c} \right)^2 \; \frac{r_4^2}{\sqrt{24}}\, Y_{2+}^{o,-1}(\Gamma_4) \; .$$

Here for the $v_1^{\pm 1}$ term of $\mathcal{E}_2(\vec{r}_4)$ we need the coefficient of

$$- \left(\frac{W_1}{\hbar c} \right)^2 \frac{1}{a_3} \; \frac{a^2}{\sqrt{24}} \; v_1^{\pm 1} \; Y_{2+}^{\mp 1,-1}(\Gamma) \; ,$$

which by sec. III.3.3(3) is:

$$\pm\, ib = \pm \frac{4}{\sqrt{6}}\, P_2^{o,\mp 1}(\theta_4') + \left(\frac{1}{4} \pm \frac{1}{4\sqrt{3}} \right) \sqrt{6}\, P_2^{-1,\mp 1}(\theta_4') + \left(\frac{1}{4} \mp \frac{1}{4\sqrt{3}} \right) \sqrt{6}\, P_2^{1,\mp 1}(\theta_4')$$

$$b = \frac{5}{3\sqrt{2}} \; .$$

In the computation of B^m_4 , these terms do not (as before) cancel, but add on account of the minus sign in Ψ^m_{3-} .

The important part of the $v_1^{\pm 1}$ term of $\mathcal{E}_2$ will then have an angular dependence proportional to $Y^{\mp 1,-1}_{2+}$ which will multiply Ψ^{1-m}_{1-} to give a term proportional to $Y^{\mp 1,-1}_{2+}\ Y^{\mp 1,m}_{1-}$. For these products, we use the Clebsch-Gordon expansion

$$Y^{k,m}_{j,p}\ Y^{k',m'}_{j',p'} = \sum_{J=|j-j'|}^{|j+j'|} Y^{k+k',m+m'}_{J,pp'}\ C^{jj'J}_{k,k',k+k'}\ C^{jj'J}_{m,m',m+m'}$$

and need the terms proportional to $Y^{\mp 2,m-1}_{3-}$, or

$$C^{213}_{-1,-1,-2}\ C^{213}_{-1,m,m-1} \quad \text{and} \quad C^{213}_{1,1,2}\ C^{213}_{-1,m,m-1}$$

which are equal. The terms arising from v_1^o cannot yield a finite result since there is no way of forming $Y^{\pm 2,m-1}_{3-}$ out of $Y^{\{o,\pm 1\},-1}_{2+}$ $Y^{o,m}_{1-}$.

Hence

$$B^m_4 = -\left(\frac{W_{13}a}{\hbar c}\right)^2 \frac{1}{\alpha_3\sqrt{24}}\ \frac{2}{7}\cdot\frac{1}{2}\cdot\sqrt{7}\ C^{213}_{112}\ C^{213}_{-1,m,m-1}\cdot ib$$

and

$$\sum_m |B^m{}_4|^2 = {\frac{W_{13}a}{\hbar c}}^{4}\ \frac{1}{168}\ \frac{1}{\alpha_3^2}\ |C^{213}_{112}|^2\ b^2 \sum_{m=-1}^{1} |C^{213}_{-1,m,m-1}|^2 .$$

Using

$$\sum_{m'=-j'}^{j'} |C^{jj'J}_{m,m',m+m'}|^2 = \frac{2J+1}{2j+1}$$

and

$$b^2 = \frac{25}{18}\ ; \qquad |C^{213}_{112}|^2 = \frac{2}{3}\ ; \qquad \sum_m |C^{213}_{-1,m,m-1}|^2 = \frac{7}{5}$$

$$|B_4^m|^2 = \frac{5}{8 \times 81} \quad \frac{W_{13}a}{\hbar c} \; \frac{1}{a_3^2}$$

and

$$\omega_{13} = \frac{2^9}{3} \times \frac{5}{2^3 \times 3^4} \cdot \frac{e^2}{\hbar c} \cdot \frac{1}{a_3^2} \left(\frac{W_{13}a}{\hbar c}\right)^4 \; \frac{W_{13}}{m_o c^2} \quad \frac{m_o c^2}{\hbar}$$

$$\frac{1}{a_3^2} = \frac{1}{9} \; \frac{W_3}{w_3} \left(\frac{W_{13}a}{\hbar c}\right)^2 = \frac{9}{4} \; \frac{W_{13}}{Mc^2} \quad \frac{W_{13}}{W_3}$$

$$w_3 = 4.91 \text{ Mev}, \qquad W_{13} = 7.21 - 6.14 = 1.07 \text{ Mev.}$$

$$\omega_{13} = \frac{20}{27} \left(\frac{e^2}{\hbar c}\right) \; \frac{W_{13}}{w_3} \; \frac{W_{13}}{W_3} \left(\frac{W_{13}}{Mc^2}\right)^2 \frac{W_{13}}{m_o c^2} \quad \frac{m_o c^2}{\hbar}$$

$$\tau_{13} = \left(\frac{27}{20}\right) (137) \left(\frac{4.91}{1.07}\right)\left(\frac{6.14}{1.07}\right)\left(\frac{4 \times 931}{1.07}\right)^2 \left(\frac{.511}{1.07}\right) \times 1.285 \times 10^{-21} \text{ sec}$$

$$\tau_{13} = 3.7 \times 10^{-11} \text{ sec.}$$

which fixes an upper limit for the lifetime of the 1^- state as $\tau_{1o} < 5 \times 10^{-13}$ sec. which is less than the previous estimate of $\tau_{1o}^{(3)} = 1.6 \times 10^{-11}$ sec.

(2) $\underline{2^- \rightarrow 3^+}$

We have noted that in all the matrix elements so far calculated the expression for the rate of an (l)th order transition can be written as a product of

a fraction $\sim \frac{2}{3} \rightarrow \frac{1}{20}$

a term $\frac{W}{w_i} \left(\frac{W}{W_2}\right)^{l-1} \left(\frac{W}{Mc^2}\right)^l \quad \frac{W}{m_o c^2}$,

where w_i corresponds to $\frac{1}{a_i^2}$

a constant factor $(\frac{e^2}{\hbar c})$ $\frac{m_o c^2}{\hbar}$.

Hence we should expect that, within a factor of approximately 6, on identification (b)

$$\frac{\tau_{1o}}{\tau_{23}} = \frac{\omega_{23}}{\omega_{1o}} \sim \left(\frac{W_{23}}{W_1}\right)^3 \cdot \frac{w_3}{w_2} = (\frac{.77}{7.12})^3 \cdot \frac{4.91}{3.84} = 1.1 \times 10^{-3}$$

hence for a lower limit

$$\tau_{1o} > 1.1 \times 10^{-3}\ \tau_{23} = 200 \times 1.1 \times 10^{-3}\ \tau_{2o} = 4 \times 10^{-16} \text{sec.}$$

and we then obtain on identification (b)

$$4 \times 10^{-16} \text{ sec.} < \tau_{1o} < 5 \times 10^{-13} \text{ sec.}$$

On identification (a)

$$\frac{\tau_{1o}}{\tau_{23}} = \left(\frac{W_{2'3}}{W_{1'}}\right)^3 = (\frac{.87}{7.01})^3 = 1.9 \times 10^{-3}$$

$$\tau_{1o} > 200 \times 1.9 \times 10^{-3}\ \tau_{2'o} = 9 \times 10^{-15} \text{sec.}$$

and

$$9 \times 10^{-15} \text{ sec.} < \tau_{1o} < 5 \times 10^{-13} \text{ sec.}$$

The above limits on the lifetime would correspond to a Ψ_{1-} wave function which is a mixture of a single particle state/α-particle state in the ratio $10^{-2}/1$ to $10^{-3}/1$ or in terms of expectation values, to a probability of 10^{-7} to 10^{-5} of finding a proton outside an α-particle.

5. Decay of the 0^+ Excited State.

The 0^+ excited state is known to decay primarily by pair production. Two quantum emission is also possible, however, and will be treated first.

5.1. Two Quantum Emission.

Let

$\vec{A}_1, \vec{A}_2$ = vector potentials for the two photons, with

$\vec{e}_1, \vec{e}_2$ = respective polarization, and

E_1, E_2 = energies

$\vec{K}_1 = \frac{E_1}{c}\hat{k}_1$, $\vec{K}_2 = \frac{E_2}{c}\hat{k}_2$ = momenta

$d\Omega_1, d\Omega_2$ = solid angles

ρ = density of states.

Fixing the energy E_2, we have for the density of states:

$$d\rho = \frac{E_1^2\, E_2^2\, dE_1\, d\Omega_1\, d\Omega_2}{(2\pi\hbar c)^6} .$$

Integrated over all $d\Omega_2$,

$$d\rho = \frac{4\pi E_1^2\, E_2^2\, dE_1\, d\Omega_1}{(2\pi\hbar c)^6}$$

considering $\hat{k}_1 = \hat{k}$ and integrating over $d\phi_1$

$$d\rho = \frac{8\pi^2}{(2\pi\hbar c)^6} E_1^2\, E_2^2\, dE_1\, d(\cos\theta_1) .$$

The perturbation Hamiltonian is

$$\mathcal{H}_2 = \frac{2Z^2e^2}{2Mc^2}(\vec{A}_1 \cdot \vec{A}_2) = \frac{Z^2e^2(4\pi c^2\hbar^2)}{Mc^2} \sum_j \hat{e}_1 \cdot \hat{e}_2 \exp[-\frac{i}{\hbar}(\vec{K}_1+\vec{K}_2)\cdot\vec{r}_j]$$

and in order to produce a transition $0^+ \rightarrow 0$, the second order term in the expansion of the exponential is required.

$$\mathcal{H}_2^{(1)} = \frac{4\pi Z^2}{Mc^2}\left(\frac{e^2}{\hbar c}\right)(\hbar c)^3 \sum_{j=1}^{4} \frac{-1}{2\hbar^2}\left[(\vec{K}_1 + \vec{K}_2)\cdot\vec{r}_j\right]^2 \hat{e}_1 \cdot \hat{e}_2$$

The transition rate into energy dE_1, angle $d\theta_1$ is

$$d\omega = \frac{2\pi}{\hbar}\cdot\frac{1}{4E_1E_2}\,\frac{8\pi^2 E_1^2 E_2^2\, dE_1\, d(\cos\theta_1)}{(2\pi\hbar c)^6}\,\frac{4\pi Z^2}{Mc^2}{}^2\,\frac{e^2}{\hbar c}{}^2\,(\hbar c)^6$$

$$\times \sum_{\text{polarizations } 1+2}\left|\langle 0,0\right|\sum_j \frac{\left[(\vec{K}_1+\vec{K}_2)\cdot\vec{r}_j\right]^2}{2\hbar^2}\,\hat{e}_1\cdot\hat{e}_2\left|0',0\rangle\right|^2 .$$

We can remove a factor $(\hat{e}_1\cdot\hat{e}_2)^2$ from the matrix element, and if we call θ_j = angle between $\vec{r}_j$ and $(\vec{K}_1 + \vec{K}_2)$, then since the wave functions are spherically symmetric,

$$|\langle|\sum_j\left[(\vec{K}_1+\vec{K}_2)\cdot\vec{r}_j\right]^2|\rangle|^2 = |\vec{K}_1+\vec{K}_2|^4\,(\cos^2\theta_j)_{av}^2\,|\langle|\sum_j r_j^2|\rangle|^2$$

but

$$(\cos^2\theta_j)_{av} = \frac{1}{3}\ .$$

The $\sum_j$ in the matrix element produces a factor 2^4, and so, putting in $Z = 2$

$$\frac{1}{\hbar^2}|\vec{K}_1 + \vec{K}_2|^2 = \frac{1}{\hbar^2 c^2}(E_1^2 + E_2^2 + 2E_1\,E_2\cos\theta_1)$$

$$d\omega = \frac{2^7}{9\pi}\left(\frac{e^2}{\hbar c}\right)^2\frac{E_1\,E_2}{(Mc^2)^2}\,\frac{dE_1}{\hbar}\,\frac{(E_1^2 + E_2^2 + 2E_1\,E_2\cos\theta_1)^2}{(\hbar c)^4}$$

$$\times \sum_{\text{polarizations}}(\hat{e}_1\cdot\hat{e}_2)^2\,d(\cos\theta_1)\,|\langle|r_4^2|\rangle|^2$$

now

$$\sum_{\text{polarizations}}(\hat{e}_1\cdot\hat{e}_2)^2 = 1 + \cos^2\theta_1\ .$$

Integrating over $d(\cos\theta_1)$

$$d\omega = \frac{2^7}{9\pi}\left(\frac{e^2}{\hbar c}\right)^2 \frac{E_1\ E_2}{(Mc^2)^2} \quad \frac{\frac{8}{3}(E_1^2 + E_2^2)^2 + \frac{64}{15} E_1^2\ E_2^2}{(\hbar c)^4} \quad \frac{dE_1}{\hbar}\ |<|r_4^2|>|^2 \ .$$

Putting

$$|<|r_4^2|>|^2 = \frac{2a^4}{\alpha_1^2} = \frac{9}{8}\ \frac{(\hbar c)^4}{(Mc^2)^2\ W_o\ W_3}$$ and integrating $\int_o^{W_o} dE_1$

we obtain the total transition rate for two-quantum emission:

$$\omega = \frac{176 \times 4}{225\pi} \times \left(\frac{e^2}{\hbar c}\right)^2 \times \frac{W_o}{W_3} \times \left(\frac{W_o}{Mc^2}\right)^4 \frac{W_o}{m_o c^2} \quad \frac{m_o c^2}{\hbar}$$

and a mean life for this process

$$\tau = \frac{1}{\omega} = \frac{225\pi}{176 \times 4} \times (137)^2 \times \frac{6.14}{6.06} \times (\frac{4 \times 937}{6.06})^4 \times \frac{.511}{6.06}$$

$$\times\ 12.85 \times 10^{-21} \text{ sec.}$$

$$\tau = 3 \times 10^{-7} \text{ sec.}$$

5.2. Pair Emission.

In the Feynman reversed time formulation [13], pair emission is the scattering of an electron from a reversed time (positron) state into normal time (electron) state. The 0' → 0 pair transition occurs through the production of an oscillating electromagnetic field (the matrix element of the nuclear electromagnetic potential) which in turn brings about the scattering (pair emission).

The electron and positron must be treated relativistically, but the nucleus can be treated non-relativistically.

Consider the pair production process first.

Notation: units are chosen so that $\hbar = c = 1$

$E_1, \vec{p}_1$ = energy, momentum four vector of positron

$E_2, \vec{p}_2$ = energy, momentum four vector of electron

$\vec{p} = \vec{p}_1 + \vec{p}_2$= total momentum imparted to the pair

$E_1 + E_2$= total energy imparted to the pair.

Since we can neglect the nuclear recoil energy,

$E_1 + E_2 = W_1$ = the excitation energy of the 0' state.

$V(\vec{p}), \vec{A}(\vec{p})$ = four vector potential for electromagnetic field which produces pairs.

The Dirac Hamiltonian for the interaction between an electron and an E.M. field is

$$\mathcal{H} = e\not{A},$$

where for any four vector

$B_\mu \equiv B_x, B_y, B_z, B_t \equiv B_t, \vec{B}$, the notation

$$\not{B} = \sum_{\mu,\nu=1}^{4} B_\mu \gamma_\nu \delta_{\mu\nu}$$

$$\delta_{\mu\nu} = \begin{cases} -1, & \mu = \nu = 1,2,3 \\ +1, & \mu = \nu = 4 \\ 0, & \mu \neq \nu \end{cases}$$

and γ_μ are the four-vector form of the Dirac operators, satisfying

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2\,\delta_{\mu\nu}$$

$$\not{B} = \sum_{\mu\nu} B_\mu \gamma_\nu \delta_{\mu\nu} = B_t \ \gamma_t - \vec{B} \cdot \vec{\gamma} \ .$$

Then the relativistic Hamiltonian for the interaction between an electron and an E.M. field is

$$\mathcal{H} = e\not{A} = eV\gamma_t - eA \cdot \vec{\gamma} .$$

Since in this problem the E.M. field does not represent free photons, we may choose the gauge so that $\vec{A} = 0$. Then the interaction is simply

$$\mathcal{H} = eV\gamma_t \quad .$$

The total rate of transition is given by

$$\omega = \frac{2\pi}{\hbar} \mathop{S} \left\{ |\langle 0,2|\mathcal{H}|0',1\rangle|^2 \frac{\rho}{N} \right\} \quad ,$$

where N is the normalizing factor for the emitted particles, and in the Feynman formulation we use

$$N = (-2E_1)\ (2E_2) = -4E_1E_2 \ .$$

The density of states is

$$\rho = \frac{p_1\ p_2\ E_1\ E_2\ dE_1\ dE_2\ d\Omega_1\ d\Omega_2}{(2\pi)^6\ d(E_1 + E_2)} \quad ;$$

and assuming that the nuclear recoil energy can be neglected (nucleus considered infinitely heavy with respect to E_1 or E_2) and regarding E_1 as fixed,

$$\frac{dE_2}{d(E_1 + dE_2)} = 1.$$

Then for emission into energy dE_1 and solid angles $d\Omega_1$ and $d\Omega_2$

$$\frac{\rho}{N} = -\frac{1}{4}\ \frac{p_1\ p_2\ dE_1\ d\Omega_1\ d\Omega_2}{(2\pi)^6}$$

For the matrix sum, we note that the matrix element $\langle 0,2|\mathcal{H}|0',1\rangle$ can be broken into two parts, a nuclear and an electronic.

$$\langle 0,2|\mathcal{H}|0',1\rangle = e\ \langle 0|V|0'\rangle\ \langle 2|\ \gamma_t|1\rangle \quad .$$

We can compute the electronic matrix element best in a momentum space representation: i.e., if the nucleus imparts total momentum $\vec{p}$,

$$<0|V|0'> = V(\vec{p}) = \int V(\vec{R})\, e^{i\frac{\vec{p}\cdot\vec{R}}{\hbar}}\, d^3\vec{R}\,,$$

where

$$V(\vec{R}) = \int \Psi_o^* \sum_{j=1}^{4} \frac{Ze}{|\vec{R}-\vec{r}_i|}\, \Psi_o\, d\tau \quad .$$

Then the matrix sum over all spin states for the electron and positron can be found by spur technique:

$$\mathcal{S}<0,2|\mathcal{H}|0',1> = e^2|V(\vec{p})|^2\ \text{Spur}\ [(\not{p}_1+m)\ \gamma_t(\not{p}_2+m)\ \gamma_t]$$

here

$$\not{p}_1 = -E_1\ \gamma_t + \vec{p}_1\cdot\vec{\gamma}$$

$$\not{p}_2 = E_2\ \gamma_t - \vec{p}_2\cdot\vec{\gamma}$$

$$\text{Spur}[(\not{p}_1+m)\gamma_t(\not{p}_2+m)\ \gamma_t] = \text{Sp}[(-E_1\ \gamma_t + \vec{p}_1\cdot\vec{\gamma} + m)(E_2\ \gamma_t + \vec{p}_2\cdot\vec{\gamma} + m)]$$

$$= -4(E_1\ E_2 + \vec{p}_1\cdot\vec{p}_2 - m^2)$$

combining expressions, we get

$$\omega = \frac{2\pi e^2}{\hbar(2\pi)^6} \iiint |V(\vec{p})|^2\ (E_1E_2 + \vec{p}_1\cdot\vec{p}_2 - m^2)\ p_1p_2\ dE_1\ d\Omega_1\ d\Omega_2\ .$$

$$V(\vec{p}) = V(p) = \int_0^\infty \int_{-1}^{1} \int_0^{2\pi} V(R)\ e^{\frac{ipR\cos\theta}{\hbar}}\ d\phi\ d(\cos\theta)\ dR$$

$$= 4\pi \int_0^\infty V(R)\ \frac{\sin\frac{pR}{\hbar}}{\frac{pR}{\hbar}}\ R^2\ dR\quad .$$

Now

$$V(\vec{R}) = \int \Psi_o^* \sum_{j=1}^{4} \frac{Ze}{|\vec{R} - \vec{r}_j|} \Psi_{o'} \, d\tau .$$

However, $Z = 2$ and from the symmetry of the wave functions, $\sum_j$ gives a factor of four. Further, $V(\vec{R})$ must be spherically symmetric; hence

$$V(\vec{R}) = V(R) = 8e \left\{ \frac{1}{R} \int_{r_4=-\infty}^{R} \Psi_o^* \Psi_{o'} \, d\tau + \int_R^{\infty} \Psi_o^* \frac{1}{r_4} \Psi_{o'} \, d\tau \right\}$$

The $-\infty$ limit on the first integral and the volume element $d\tau$ are to be taken in accordance with sec. III.2.2. $V(R)$ dies off rapidly for $R > a$, and $V(2a) \sim 10^{-3} V(a)$. In forming $V(p)$, therefore, since $p < 5.5$ Mev/c (and for $R = 2a$, $\frac{pR}{\hbar} \sim \frac{1}{10}$) we can let $(\sin \frac{pR}{\hbar})/(pR/\hbar) \sim 1$ and use

$$V(p) = V = 32\pi e \sqrt{\frac{2}{\pi}} \int_0^{\infty} \int_{-\infty}^{\alpha_1(\frac{R}{a}-1)} Rq_1 \, e^{-q_1^2} \, dq_1 \, dR$$

$$+ \int_0^{\infty} \int_{\alpha_1(\frac{R}{a}-1)}^{\infty} R^2 q_1 \left[a(1 + \frac{q_1}{\alpha_1}) \right]^{-1} e^{-q_1^2} \, dq_1 \, dR$$

$$V = 32\pi e \sqrt{\frac{2}{\pi}} \, (I_1 + I_2) \quad .$$

In both I_1 and I_2 we may with little error, replace the lower limits on dR by $-\infty$.

$$I_1 = \int_{-\infty}^{\infty} - \frac{R}{2} \exp[-\alpha_1^2 \, (\frac{R}{a} -1)^2] \, dR = - \frac{1}{2} \int_{-\infty}^{\infty} (x + a) \exp[- \frac{\alpha_1^2 \, x^2}{a^2}] \, dx$$

$$= - \frac{a^2 \sqrt{\pi}}{2\alpha_1} \quad .$$

In I_2 we change the order of integration:

$$I_2 = \int_{-\infty}^{\infty} \int_{\alpha_1(\frac{R}{a}-1)}^{\infty} (\quad) \, dq_1 \, dR$$

$$= \int_{-\infty}^{\infty} \int_{0}^{a(1+\frac{q_1}{\alpha_1})} q_1 \left[a(1+\frac{q_1}{\alpha_1})\right]^{-1} e^{-q_1^2} R^2 \, dR \, dq_1$$

$$I_2 = \int_{-\infty}^{\infty} \frac{q_1}{3} \left[a(1+\frac{q_1}{\alpha_1})\right]^2 e^{-q_1^2} \, dq_1 = \frac{a^2\sqrt{\pi}}{3\alpha_1}$$

$$I_1 + I_2 = -\frac{a^2\sqrt{\pi}}{6\alpha_1}$$

$$V = -\frac{16\pi a^2 e \sqrt{2}}{3\alpha_1} .$$

Putting V into ω :

$$\omega = \frac{2^5 a^4 e^4}{9\cancel{h} \pi^3 \alpha_1^2} \iiint (E_1E_2 + \vec{p}_1 \cdot \vec{p}_2 - m^2) p_1p_2 \, dE_1 \, d\Omega_1 \, d\Omega_2$$

integrating $d\Omega_2$, putting $\vec{p}_1 \cdot \vec{p}_q = p_1p_2 \cos\theta$ and integrating $d\phi_1$:

$$\omega = \frac{2^8 a^4 e^4}{9\cancel{h} \pi \alpha_1^2} \int\int_{-1}^{1} (E_1E_2 + p_1p_2 \cos\theta - m^2) p_1p_2 \, d(\cos\theta_1) dE_1$$

integrating $d(\cos\theta)$, using the extreme relativistic approximation:

$$p_1 = E_1 , \qquad p_2 = E_2 , \qquad E_1E_2 >> m^2 ,$$

and letting $E_2 = W_1 - E_1$

$$\omega = \frac{2^9 a^4 e^4}{9\hbar \pi a_1^2} \int_o^{W_1} E_1^2 (W_1 - E_1)^2 \, dE_1$$

$$\omega = \frac{2^7}{9 \times 15} \quad \frac{a^4 e^4 W_1^5}{\hbar \pi a_1^2} \quad ;$$

putting back all $\hbar$, c terms

$$\omega = \frac{2^7}{9 \times 15} \left(\frac{e^2}{\hbar c}\right)^2 \frac{1}{\pi a_1^2} \cdot \left(\frac{aW_1}{\hbar c}\right)^4 \left(\frac{W_1}{m_o c^2}\right) \quad \frac{m_o c^2}{\hbar}$$

and with

$$\frac{1}{a_1^2} \left(\frac{aW_1}{\hbar c}\right)^2 = \frac{W_1}{4Mc^2}$$

$$\left(\frac{aW_1}{\hbar c}\right)^2 = \frac{9}{4} \quad \frac{W_1}{W_3} \quad \frac{W_1}{Mc^2}$$

$$= \frac{8}{15\pi} \left(\frac{e^2}{\hbar c}\right)^2 \quad \frac{W_1}{W_3} \left(\frac{W_1}{Mc^2}\right)^2 \quad \frac{W_1}{m_o c^2} \quad \frac{m_o c^2}{\hbar}$$

$$\tau = \frac{1}{\omega} = \frac{15\pi}{8} (137)^2 \left(\frac{6.14}{6.06}\right) \times \left(\frac{4 \times 937}{6.06}\right)^2 \times \left(\frac{.511}{6.06}\right) \times 1.285 \times 10^{-21} \text{ sec.}$$

$$\tau = 4.6 \times 10^{-12} \text{ sec.}$$

6. Comparison with Experiment.

The experimental and theoretical mean lives for the four lowest excited energy levels are summarized on the following page.

Mean Life in Seconds.

State	Energy (Mev)	Experimental	Ref.	Theoretical	Remarks
0^+	6.06	$7\pm1\text{x}10^{-11}$	[14]	$4.6\text{x}10^{-12}$	
3^-	6.14	$>4.3\text{x}10^{-12}$; $<1.4\text{x}10^{-11}$	[15]	$3.2\text{x}10^{-11}$	
2^+	6.91	$\leq1.7\text{x}10^{-14}$	[15]	$1.95\text{x}10^{-15}$ $2.4\ \text{x}10^{-14}$	Ident.(b) Ident.(a)
1^-	7.12	$\leq1.2\text{x}10^{-15}$	[15]	$\left\{>4\text{x}10^{-16};\ <5\text{x}10^{-13}\right\}$ $\left\{>9\text{x}10^{-15};\ <5\text{x}10^{-13}\right\}$	Ident.(b) Ident.(a)

The prediction for the 0^+ lifetime is a factor of ~ 15 too short, while that of the 3^- state is 2 or 3 times too long.

Since the α-particle model is expected to be fairly good in these computations, the discrepancies here reflect the basic inaccuracy of computation with inexact wave functions.

For the 2^+ lifetime it is apparent that identification (b) for the 2^+ state is in closer agreement with experiment than is identification (a), although the lifetime computed on identification (a) is no more discrepant than that of the 3^- state.

For the 1^- lifetime the theoretical limits are those given by the back-door approach of sec. III.4. Since the upper limit is based upon the 2^+ lifetime, the 1^- lifetime agreement with experiment is also better on identification(b) than it is on identification (a).

PART IV. APPLICATIONS TO 0^{17}

1. Approach.

The nucleus 0^{17} is known to have a ground state with $J = \frac{5}{2} +$ and a state at 870 Kev excitation with $J = \frac{1}{2} +$. The lifetime of the $\frac{1}{2} +$ state has been measured by Thirion and Telegdi [16] and found to be $2.5 \pm 1 \times 10^{-10}$ sec.

On the strict shell model, 0^{17} is expected to consist of a single neutron outside of a core of 0^{16} in the ground state. In the ground state, the neutron is in a $d_{5/2}$ state, while in the excited state, it is in an $s_{1/2}$ state. On such a model, assuming a radius of $1.5A^{1/3} \times 10^{-13}$ cm $(A = 17)$, these authors [16] find a lifetime of $\sim 10^{-7}$ sec.

They then depart from the strict shell model, assuming an admixture of excited core state (0^{16} in the 2^+ state) and find that upon assumption of a transition rate for $2^+ \rightarrow 0^+$ in 0^{16} which is 20 times that $(1.25 \times 10^{10}\ \text{sec}^{-1})$ for a single proton transition in 0^{16}, then a 2 per cent probability of finding 0^{16} is sufficient to account for the observed lifetime of the $\frac{1}{2} +$ state, and is still consistent with the measured quadrupole moment [17], $- .005 \pm .002\ e \times 10^{-24}\ \text{cm}^2$.

In this section we perform similar calculations, using the α-particle model to describe the 0^{16} core. We find that we can obtain agreement with the observed lifetime of the $\frac{1}{2} +$ state on identification (b) for the 2^+ state of 0^{16}, but that the electric quadrupole and magnetic moment of the ground state will be of slightly lower magnitude than observed values.

2. The Wave Functions.

We assume that, as a result of some unspecified effective potential between the neutron and the 0^{16} core, the two states of 0^{17} can be represented by:

$$\Psi^m_{5/2}(0^{17}) = a_o \Phi^m_{d_{5/2}}(n)\ \Psi_o(0^{16}) + a_2 \sum_{j=-1/2}^{1/2} C^{1/2,2,5/2}_{j,m-j,m}\ \Phi^j_{s_{1/2}}(n)\ \Psi^{m-j}_{2+}(0^{16})$$

$$\Psi^m_{1/2}(0^{17*}) = b_o \Phi^m_{s_{1/2}}(n)\ \Psi_o(0^{16}) + b_2 \sum_{j=-5/2}^{5/2} C^{5/2,2,1/2}_{j,m-j,m}\ \Phi^j_{d_{5/2}}(n)\ \Psi^{m-j}_{2+}(0^{16}) ,$$

where

a_o, a_2, b_o, b_2 are parameters whose values are to be found

$$|a_o|^2 + |a_2|^2 = |b_o|^2 + |b_2|^2 = 1 .$$

To be more specific, we employ the same coordinates as before for 0^{16}

$q_1 \cdots q_6$ = internal coordinates of 0^{16}

Γ = angular coordinates of 0^{16}

and use

ρ, θ, ϕ = radius and angular coordinates for the relative motion.

Hereafter we shall suppress the arguments 0^{16}, n, 0^{17}, s, d and use ρ and q as shorthand for ρ, θ, ϕ and $q_1 \cdots q_6$, Γ respectively.

The wave functions Ψ_o and Ψ_2, and $\Phi_{1/2}$ and $\Phi_{5/2}$ are orthonormal.

3. Operators.

There are three operations which we shall employ.

For the lifetime calculation we need the electric quadrupole operator:

$$\mathcal{E}_2 = -\left(\frac{W}{\hbar c}\right)^2 \frac{1}{\sqrt{24}} \sum_{\text{charges}\, i} Z_i\, r_i^2 [Y_{2+}^{o,-1}(\Gamma_i) - Y_{2+}^{o,1}(\Gamma_i)] \; .$$

For the magnetic moment calculation, we need the magnetic moment operator

$$\mu = \sum_{\text{particles } i} [\, \mu_i + \frac{\hbar Z_i\, e_i}{m_i\, c}\, (\vec{J}_i)_z \,] .$$

For the electric quadrupole moment calculation we need the electric quadrupole moment operator

$$Q = \sum_{\text{particles}\, i} eZ_i(3Z_i^2 - r_i^2) \; .$$

Each of these operators may be separated rigorously into a linear sum of an operator which acts only on the internal coordinates of 0^{16} and one which acts only on the relative motion (for μ, also the neutron spin)*.

---

* $\mathcal{E}_2$ and Q are bilinear forms in the cartesian coordinates $x_{j\alpha}$ of the α-particles (subscript j designates particle, α the component) and may be written in the form

$$Op = \sum_{\alpha,\beta} \sum_j C_{\alpha\beta}\, x_{j\alpha}\, x_{j\beta} \quad ,$$

but

$$x_{j\alpha} = r_{j\alpha} + \gamma \rho_\alpha \qquad\qquad (\gamma = \frac{1}{16} \text{ here}) ,$$

where

$r_{j\alpha}$ = the internal coordinate

ρ_α = separation coordinate

$$Op = \sum_{\alpha,\beta} C_{\alpha\beta} \sum_j (r_{j\alpha} + \gamma\rho_\alpha)(r_{j\beta} + \gamma\rho_\beta)$$

and the cross terms vanish by virtue of $\sum_j r_{j\alpha} = 0$.

$$Op = \sum_{\alpha,\beta} C_{\alpha\beta}(4\gamma^2\, \rho_\alpha\rho_\beta + \sum_j r_{j\alpha}\, r_{j\beta}) .$$

A similar argument applies to μ . The term μ_i works only on the neutron spin, and $(J_i)_z$ is bilinear form in the coordinates and momenta, and the proof will hold by virtue of $\sum_j p_{j\alpha} = 0$.

(1) Electric Quadrupole Operator.

$$\mathcal{E}_2 = \mathcal{E}_2(q) + \mathcal{E}_2(\rho)$$

where

$$\mathcal{E}_2(q) = \frac{-8}{\sqrt{24}} \left(\frac{W}{\hbar c}\right)^2 r_4^2 \, [Y_{2+}^{0,-1}(\Gamma_4) - Y_{2+}^{0,1}(\Gamma_4)]$$

$$\mathcal{E}_2(\rho) = \frac{8}{\sqrt{24}} \left(\frac{W}{\hbar c}\right)^2 \frac{1}{(16)^2} \rho^2 [Y_{2+}^{0,-1}(\theta,\phi) - Y_{2+}^{0,1}(\theta,\phi)]$$

(note that $\mathcal{E}_2(q)$ differs from our definition of $\mathcal{E}_2$ in sec. III.3.2.1 by a factor of 8).

(2) Magnetic Moment Operator.

$$\mu = \mu(q) + \mu(\rho) + \mu(s)$$

where if we call

J = total angular momentum

I = angular momentum of 0^{16}

L = angular momentum of relative motion

S = angular momentum of neutron

μ_0 = nuclear magneton.

$$\mu(q) = g_I \, m_J \frac{\vec{I}\cdot\vec{J}}{|J|^2} \mu_0 \qquad g_I = \frac{1}{2} = \text{gyromagnetic ratio of an } \alpha\text{-particle}$$

$$\mu(\rho) = g_L \, m_J \frac{\vec{L}\cdot\vec{J}}{|J|^2} \mu_0 \qquad g_L = \frac{8}{241} = \text{g.m. ratio for relative motion.}$$

g_L comes about from reduced mass consideration. For an angular velocity ω, classically, (M_0 = nucleon mass).

$$\hbar L = \omega\rho^2 M_o \left(\frac{16}{(16)^2} + \left(\frac{15}{16}\right)^2\right) = \omega\rho^2 M_o \cdot \frac{241}{(16)^2}$$

$$\mu_L = \frac{\omega\rho^2}{2} \cdot \frac{8e}{c} \frac{1}{(16)^2}$$

$$g_L = \frac{\mu_L}{L\,\mu_o} = \frac{8e\hbar}{241\ m_o c}{}_o = \frac{8}{241}$$

$$(s) = g_s\, m_J \frac{\vec{S}\cdot\vec{J}}{|J|^2} \mu_o \qquad g_s = -1.913 \times 2 \quad .$$

(3) Quadrupole Moment Operator.

$$Q = Q(q) + Q(\rho)$$

$$Q(q) = 16e\ r_4^2\ Y_{2+}^{oo}(\Gamma_4)$$

$$Q(\rho) = \frac{16e}{256} \rho^2\ P_2^{oo}(\theta) \quad .$$

4. Computation of lifetime of the $\frac{1}{2}+$ State.

We shall use in the calculations only that part of $\mathcal{E}_2$ which lowers the value of m. Then

$$\omega = \frac{2^3}{2} \left(\frac{e^2}{\hbar c}\right) \frac{W}{\hbar} \sum_{m=-1/2}^{1/2} |B^m|^2$$

where

$$B^m = <\frac{5}{2}, m-1 | \mathcal{E}_2 | \frac{1}{2}, m> \quad .$$

We shall choose the phase of wave functions so that a_o and b_o are both real.

Then

$$B^m = a_o\, b_o(\Phi^{m-1}_{5/2} ,\ \mathcal{E}_2(\rho)\ \Phi^{m}_{1/2})$$

$$+ a_2^*\, b_2 \sum_{j=-1/2}^{1/2} C^{1/2,2,5/2}_{j,m-1+j,m-1}\ C^{5/2,2,1/2}_{j+1,m-1+j,m}\ (\Phi^{j}_{1/2} ,\ \mathcal{E}_2(\rho)\ \Phi^{j+1}_{5/2})$$

$$+ a_o\, b_2\, C^{5/2,2,1/2}_{m-1,1,m}\ (\Psi^o_o ,\ \mathcal{E}_2(q)\ \Psi^1_2)$$

$$+ a_2^*\, b_o\, C^{1/2,2,5/2}_{m,-1,m-1}\ (\Psi^{-1}_2 ,\ \mathcal{E}_2(q)\ \Psi^o_o)\ .$$

Only the latter two terms will contribute significantly to B^m. Further

$$C^{abc}_{\alpha\beta\gamma} = \sqrt{\frac{2c+1}{2a+1}}\ (-1)^{a-\alpha+c-\gamma}\ C^{cba}_{\gamma,-\beta,\alpha}$$

so

$$C^{5/2,2,1/2}_{m-1,1,m} = \frac{\sqrt{2}}{\sqrt{6}}\ (-1)^{4-2m}\ C^{1/2,2,5/2}_{m,-1,m-1} = -\frac{1}{\sqrt{3}}\ C^{1/2,2,5/2}_{m,-1,m-1}$$

and

$(\Psi^{-1}_2 , \mathcal{E}_2(q)\ \Psi^o_o) = -\ (\Psi^o_o , \mathcal{E}_2(q)\ \Psi^1_2)$, since $\mathcal{E}_2(q)$ is a real function (and hence a Hermitian operator), and since

$$(\Psi^o_o)^* = \Psi^o_o \quad \text{but} \quad \Psi^{-1}_2 = -\ (\Psi^1_2)^*\ .$$

We therefore obtain

$$B^m = \frac{1}{\sqrt{3}}\ (a_o b_2 + \sqrt{3}\ b_o a_2^*)\ C^{1/2,2,5/2}_{m,-1,m-1}\ (\Psi^o_o , \mathcal{E}_2(q)\ \Psi^1_2)$$

and using

$$\sum_{\alpha=-a}^{a} |C^{abc}_{\alpha,\beta,\alpha+\beta}|^2 = \frac{2c+1}{2b+1}$$

and

$$(\Psi^o_o ,\ \mathcal{E}_2(q)\ \Psi^1_2) = 8\ (\frac{W}{W_2})^2\ B_2$$

(B_2 and W_2 are associated with identification (b) for the 2^+ state; on identification (a) they would be replaced by B_2' and W_1' respectively.) Therefore, we obtain

$$\sum_m |B^m|^2 = \frac{1}{3} \cdot \frac{6}{5} \cdot 2^6 \, |a_o b_2 + \sqrt{3}\, b_o a_2^*|^2 \left(\frac{W}{W_2}\right)^4 |B_2|^2$$

and a transition rate

$$\omega = |a_o b_2 + \sqrt{3}\, b_o\, a_2^*|^2 \left(\frac{W}{W_2}\right)^5 \omega_{2o}$$

$$W = .870 \text{ Mev.}$$

Using identification (b) for the 2^+ state of O^{16}

$$W_2 = 6.91 \text{ Mev.}, \qquad \omega_{2o} = 5.14 \times 10^{14} \text{ sec}^{-1}.$$

$$\omega_b = |a_o b_2 + \sqrt{3}\, b_o\, a_2^*|^2 \times 1.6 \times 10^{10} \text{sec}^{-1} \; .$$

Using identification (a):

$$W_1' = 7.01 \text{ Mev.} \qquad \omega_{2o}' = 4.2 \times 10^{13} \text{ sec}^{-1}$$

$$\omega_a = |a_o b_2 + \sqrt{3}\, b_o a_2^*|^2 \times 1.2 \times 10^{9} \text{ sec}^{-1} \; .$$

5. Magnetic Dipole Moment.

The magnetic dipole moment is defined as the expectation value of the magnetic dipole operator in the $\Psi^{5/2}_{5/2}$ state.

$$\mu = |a_o|^2 \left(\Phi^{5/2}_{5/2} \, , [\mu(\rho) + \mu(s)] \quad {}^{5/2}_{5/2}\right)$$

$$+ \; |a_2|^2 \left(C^{1/2,2,5/2}_{1/2,2,5/2}\right) \left[\left(\Psi^2_2, \mu\,(q) \Psi^{-2}_2\right) + \left(\Phi^{1/2}_{1/2}, \mu\,(s)\; \phi^{1/2}_{1/2}\right)\right]$$

in the first term, $\vec{I} = 0$ and $\vec{J} = \vec{L} + \vec{S}$ where $L = 2$, $S = 1/2$; in the second, $L = 0$ and $\vec{J} = \vec{I} + \vec{S}$ with $I = 2$, $S = 1/2$

$$\frac{\mu}{\mu_o} = |a_o|^2 \left(\frac{8}{241} \quad \frac{\vec{L} \cdot \vec{J}}{(J + 1)} - 2 \text{ x } 1.913 \, \frac{\vec{S} \cdot \vec{J}}{(J + 1)} \right)$$

$$+ |a_2|^2 \, (C^{1/2,2,5/2}_{1/2,2,5/2}) \, (\frac{1}{2} \, \frac{\vec{I} \cdot \vec{J}}{J + 1} - 2 \cdot 1.913 \, \frac{\vec{S} \cdot \vec{J}}{J + 1})$$

putting in $C^{1/2,2,5/2}_{1/2,2,5/2} = 1$ and since $J = I + S = L + S$

$$\frac{\vec{L} \cdot \vec{J}}{J + 1} = \frac{\vec{I} \cdot \vec{J}}{J + 1} = L = 2$$

$$\frac{\vec{S} \cdot \vec{J}}{J + 1} = S = \frac{1}{2}$$

$$|a_o|^2 = 1 - |a_2|^2$$

$$\frac{\mu}{\mu_o} = (1 - |a_2|^2) \, (\frac{16}{241} - 1.913) + |a_2|^2 \, (1 - 1.913 \sqrt{\frac{7}{15}})$$

$$= - 1.847 + .934 \, |a_2|^2 \ .$$

6. Electric Quadrupole Moment.

The electric quadrupole moment is defined as the expectation value of Q in the state $\Psi^{5/2}_{5/2}$

$$Q = |a_o|^2 \, (\Phi^{5/2}_{5/2}, \, Q(\rho) \, \Phi^{5/2}_{5/2}) + |a_2|^2 \, (\Psi^2_2, \, Q(q) \, \Psi^2_2) \ .$$

The first term is the neutron wave function contribution. For the wave function we can use

$$\Phi^{5/2}_{5/2} = \sqrt{\frac{5}{8\pi}} \; f_d(\rho) \, Y^{o,2}_{2+}(\theta, \phi) \; \chi^{1/2}_{1/2}$$

where

$f_d(\rho)$ is the normalized d-state radial wave function

$\chi^{1/2}_{1/2}$ is the neutron spin wave function

$\sqrt{\frac{5}{8\pi}}$ is a normalizing factor for angular integration

$$(\Phi^{5/2}_{5/2}\,,\ \frac{1}{16}\,e\,\rho^2\ P_2^{oo}(\theta)\ \ \Phi^{5/2}_{5/2}) = \frac{1}{16}\,e\ \cdot\ C^{222}_{ooo}\ C^{222}_{o22}(f_d,\rho^2\ f_d)$$

and

$$C^{222}_{ooo}\ C^{222}_{o22} = -\ \frac{2}{7}$$

$$Q(\rho) = |a_o|^2\ \cdot\ \frac{-1}{56}\,e(f_d,\rho^2\ f_d)\quad .$$

If we use

$$(f_d,\rho^2\ f_d) = (1.5\ x\ 17^{1/3}\ x\ 10^{-13}\ cm)^2$$

we get

$$Q(\rho) = |a_o|^2\ (-\ 2.7\ x\ 10^{-3}\ e\ x\ 10^{-24}\ cm^2)\quad .$$

For the second term, the contribution of the core, we shall require a second order expansion of $Q(q)$ in terms of q_1, since $P_2^{oo}(\Gamma_4^{!})$ is zero and therefore the zeroth order terms vanish.

We shall have to perform the calculation twice, first for identification (b) and second for identification (a).

Identification (b).

$$\Psi_2^2 = \sqrt{5}\ \ \sqrt{2}\ \frac{1}{2}\ \left\{\sqrt{2}\ q_3\ Y^{o,2}_{2+}(\Gamma) + q_2[Y^{2,2}_{2+}(\Gamma) + Y^{-2,2}_{2+}(\Gamma)]\right\}\ \Psi_o$$

$$Q(q) = |a_2|^2\ 16^e\ r_4^2\ Y^{oo}_{2+}(\Gamma_4)$$

and we need the terms of second order in q_3, q_2 .

$$r_4^2 = a^2\ \ \left(1 + \frac{1}{\alpha_2^2}\ [q_2^2 + q_3^2]\right)$$

$$\Gamma_4 = \Gamma_q\ \Gamma_4^{!}\ \Gamma$$

where

$$\Gamma_q = 1 - \frac{1}{2a_2^2}\,(q_2^2 + q_3^2) - \frac{q_2^2}{2a_2^2}\,(S'_x)^2 - \frac{1}{2}\,\frac{q_3^2}{a_2^2}\,(S'_y)^2 + \frac{1}{2}\,\frac{q_2 q_3}{a_2^2}\,(S'_x S'_y + S'_y S'_x)$$

$$(S'_x)^2 = \frac{1}{4}\,(S'_+ + S'_-)^2 = \frac{1}{4}\,[(S'_+)^2 + (S'_-)^2 + S'_+ S'_- + S'_- S'_+]$$

$$(S'_y)^2 = -\frac{1}{4}(S'_- - S'_+)^2 = \frac{1}{4}[-(S'_+)^2 - (S'_-)^2 + S'_+ S'_- + S'_- S'_+]$$

$$S'_x S'_y + S'_y S'_x = \frac{i}{4}\,[(S'_- - S'_+)(S'_- + S'_+) + (S'_- + S'_+)(S'_- - S'_+)] = \frac{i}{2}[(S'_-)^2 - (S'_+)^2]$$

and

$$Y_{2+}^{oo}(\Gamma'_4\;\Gamma) = \sum_{h=-2}^{2} Y_{2+}^{oh}(\Gamma'_4)\; Y_{2+}^{ho}(\Gamma)$$

$$(S'_\pm)^2 \cdot Y_{2+}^{oh}(\Gamma'_4) = 2\sqrt{6}\; Y_{2+}^{\mp 2,h}(\Gamma'_4)$$

$$(S'_+ S'_- + S'_- S'_+)\; Y_{2+}^{oh}(\Gamma'_4) = 12\; Y_{2+}^{oh}(\Gamma'_4) \quad .$$

In the h-summation, only terms with $h = \pm 2,\ 0$ are important:

$$Y_{2+}^{oo}(\Gamma'_4) = 0$$

$$Y_{2+}^{\pm 2,o}(\Gamma'_4) = \frac{1}{\sqrt{6}}$$

$$Y_{2+}^{o,\pm 2}(\Gamma'_4) = \mp\frac{i}{\sqrt{6}}$$

$$Y_{2+}^{2,\pm 2}(\Gamma'_4) + Y_{2+}^{-2,\pm 2}(\Gamma'_4) = \mp\;\frac{2i}{3}$$

$$Y_{2+}^{2,\pm 2}(\Gamma'_4) - Y_{2+}^{-2,\pm 2}(\Gamma'_4) = -\frac{i}{\sqrt{3}}$$

to second order:

$$r_4^2\, Y_{2+}^{oo}(\Gamma_4) = \frac{a^2}{\alpha_2^2} \left\{ [-\frac{1}{2} q_2^2 + \frac{1}{2} q_3^2]\, Y_{2+}^{oo}(\Gamma) \right.$$

$$+ \quad i\, \frac{\sqrt{6}}{3} q_2^2 + i\, \frac{\sqrt{6}}{12} q_3^2 + \frac{1}{\sqrt{2}} q_2 q_3 \quad Y_{2+}^{2,o}(\Gamma)$$

$$\left. + \quad -i\, \frac{\sqrt{6}}{3} q_2^2 - i\, \frac{\sqrt{6}}{12} + \frac{1}{\sqrt{2}} q_2 q_3 \quad Y_{2+}^{-2,o}(\Gamma) \right\} \quad .$$

In the matrix element, only the $q_2 q_3$ terms can survive, since in the Y_2^{oo} term the q_2^2 contribution will cancel that of q_3^2, while in the other terms the $q_2^2\, Y_2^{2o}$ and $q_3^2\, Y_2^{2o}$ will cancel the $q_2^2\, Y_2^{-2o}$ and $q_3^2\, Y_2^{-2o}$ contributions, respectively. Using $C^{222}_{\pm2,o,\pm2} = C^{222}_{\pm2,\mp2,o} = \sqrt{\frac{2}{7}}$, we obtain

$$Q(q) = 16e\, \frac{a^2}{\alpha_2^2} \cdot \frac{10}{4} \cdot \frac{1}{4} \cdot \frac{1}{5} \cdot \frac{1}{\sqrt{2}} \cdot 4\sqrt{2} \cdot \frac{2}{7} = \frac{16}{7}\, e\, \frac{a^2}{\alpha_2^2}\, |a_2|^2 \quad .$$

$$\frac{a^2}{\alpha_2^2} = \frac{1}{4} \left(\frac{\hbar}{2M_o c}\right)^2 \cdot \frac{m_o c^2}{w_2} \qquad (M_o = \text{proton mass})$$

$$Q(q) = |a_2|^2\ \frac{4}{7} \cdot \frac{937}{3.84}\ \text{x}\ e\ \text{x}\ 1.11\ \text{x}\ 10^{-28}\ \text{cm}^2 = |a_2|^2\ \text{x}\ 1.5e\ \text{x}\ 10^{-26}\text{cm}^2$$

hence on identification (b),

$$Q_b = (-.27 + 18|a_2|^2)\ e\ \text{x}\ 10^{-27}\ \text{cm}^2 \quad .$$

<u>Identification (a).</u>

$$\Psi^2_{2+'} = \sqrt{5}\ \sqrt{2}\ \frac{1}{\sqrt{6}} \left\{ \sqrt{2}\ v_1^1\ Y_{2+}^{-1,2}(\Gamma) + v_1^o[Y_{2+}^{2,2} - Y_{2+}^{-2,2}(\Gamma)] \right.$$

$$\left. - \sqrt{2}\ v_1^{-1}\ Y_{2+}^{1,2}(\Gamma) \right\} \quad \Psi_o \quad ;$$

$$Q'(q) = |a_2|^2 \cdot 16e\ r_4^2\ Y_{2+}^{oo}\ (\Gamma_4) \quad .$$

We need terms to second order in q_4, q_5, q_6

$$r_4^2 = a_2 \left\{ 1 + \frac{4}{a_3\sqrt{6}} (q_4 + q_5 + q_6) + \frac{1}{a_3^2} (q_4 + q_5 + q_6)^2 - \frac{1}{a_3^2} (q_4 q_5 + q_4 q_6 + q_5 q_6) \right\} \quad ;$$

$$\Gamma_4 = \Gamma_q \Gamma_4' \Gamma \quad ;$$

where

$$\Gamma_q = 1 - \frac{1}{6a_3^2} (q_4 + q_5 + q_6)^2 + \frac{1}{2a_3^2} (q_4 q_5 + q_4 q_6 + q_5 q_6)$$

$$+ \left[1 - \frac{2}{a_3\sqrt{6}} (q_4 + q_5 + q_6) \right] \left[\frac{-i}{2a_3} (q_4 - q_5) S_x' + \frac{i}{2a_3\sqrt{3}} (2q_6 - q_4 - q_5) S_y' \right]$$

$$- \frac{1}{8a_3^2} (q_4 - q_5)^2 (S_x')^2 - \frac{1}{24a_3^2} (2q_6 - q_4 - q_5)^2 (S_y')^2$$

$$+ \frac{1}{8a_3^2\sqrt{3}} (q_4 - q_5)(2q_6 - q_4 - q_5)(S_x' S_y' + S_y' S_x') \quad .$$

To second order:

$$\frac{a_3^2 r_4^2}{a^2} \Gamma_q = - \frac{5}{3} v_1^1 v_1^{-1} - \frac{7i}{12} [(v_1^1)^2 - (v_1^{-1})^2] + \frac{1}{6} v_1^o (e^{3\pi i/4} v_1^1 - e^{-3\pi i/4} v_1^{-1})$$

$$+ \frac{5}{6} (v_1^o)^2 + \frac{i}{\sqrt{6}} [(v_1^1)^2 + (v_1^{-1})^2 + v_1^o (e^{-3\pi i/4} v_1^1 - e^{3\pi i/4} v_1^{-1})] S_x'$$

$$- \frac{i}{3\sqrt{2}} [i(v_1^1)^2 + 2v_1^1 v_1^{-1} - i(v_1^{-1})^2 + v_1^o (e^{3\pi i/4} v_1^1 - e^{-3\pi i/4} v_1^{-1}) + 2(v_1^o)^2] S_y'$$

$$- \frac{1}{8} [i(v_1^1)^2 + 2v_1^1 v_1^{-1} - i(v_1^{-1})^2] (S_x')^2$$

$$- \frac{1}{24} [-i(v_1^1)^2 - 2v_1^1 v_1^{-1} + i(v_1^{-1})^2 - 4v_1^o (e^{3\pi i/4} v_1^1 - e^{-3\pi i/4} v_1^{-1}) + 4(v_1^o)^2] (S_y')^2$$

$$+ \frac{1}{8\sqrt{3}} [-(v_1^1)^2 - (v_1^{-1})^2 + 2v_1^o (e^{-3\pi i/4} v_1^1 - e^{3\pi i/4} v_1^{-1})] (S_x' S_y' + S_y' S_x') \quad .$$

$$Y_{2+}^{oo}(\Gamma_4) = \sum_{h=-2}^{2} Y_{2+}^{oh}(\Gamma_q \, \Gamma_4') \; Y_{2+}^{ho}(\Gamma)$$

$$S_x' = \frac{1}{2} \, (S_-' + S_+')$$

$$S_y' = \frac{i}{2} \, (S_-' - S_+')$$

$$(S_x')^2 = \frac{1}{4}[(S_+')^2 + (S_-')^2 + (S_+'S_-' + S_-'S_+')]$$

$$(S_y')^2 = - \frac{1}{4} \, [(S_+')^2 + (S_-')^2 - (S_+'S_-' + S_-'S_+')]$$

$$S_x'S_y' + S_y'S_x' = \frac{i}{2} \, [(S_-')^2 - (S_+')^2]$$

$$S_{\mp}' \; Y_{2+}^{oh}(\Gamma_4') = \sqrt{6} \; Y_{2+}^{\pm1,h}(\Gamma_4')$$

$$(S_{\mp}')^2 \; Y_{2+}^{oh}(\Gamma_4') = 2 \sqrt{6} \; Y_{2+}^{\pm2,h}(\Gamma_4')$$

$$(S_+'S_-' + S_-'S_+') \; Y_{2+}^{oh}(\Gamma_4') = 12 \; Y_{2+}^{oh}(\Gamma_4')$$

In the matrix element only the following combinations can survive:

$$v_1^1 \, v_1^{-1} \, Y_{2+}^{oo}(\Gamma), \quad (v_1^o)^2 \, Y_{2+}^{oo}(\Gamma), \quad (v_1^1)^2 \, Y_{2+}^{-2,o}(\Gamma), \quad (v_1^{-1})^2 \, Y_{2+}^{2o}(\Gamma),$$

$$v_1^o \, v_1^1 \, Y_{2+}^{1o}(\Gamma), \quad v_1^o \, v_1^{-1} \, Y_{2+}^{-1,o}(\Gamma) \; .$$

If in $\frac{\alpha_3^2}{a^2} r_4^2 \, Y_{2+}^{oo}(\Gamma_4)$ the coefficients of the above four terms are called g_1, g_2, ... , g_6, respectively, the matrix element of $r_4^2 \, Y_{2+}^{oo}(\Gamma_4)$ is:

$$(\Psi_{2+'}^2, \; r_4^2 \, Y_{2+}^{oo}(\Gamma_4) \; \Psi_{2+'}^2) = \frac{a^2}{\alpha_3^2} \, C_{o22}^{222} \; \Big\{ [- \frac{1}{3}(C_{o11}^{222} + C_{o,-1-1}^{222})$$

$$- \frac{1}{12}(C_{o22}^{222} + C_{o,-2,-2}^{222})]g_1 + [\frac{1}{6}(C_{o11}^{222} + C_{o,-1,-1}^{222}) + \frac{1}{4}(C_{o22}^{222} + C_{o,-2,-2}^{222})]g_2$$

$$+ \frac{1}{3} \, C_{-2,1,-1}^{222} \; g_3 + \frac{1}{3} \, C_{2,-1,1}^{222} \; g_4 + \frac{\sqrt{2}}{6} \, (C_{112}^{222} - C_{1,-2,-1}^{222})g_5$$

$$+ \frac{\sqrt{2}}{6} \, (C_{-1,-1,-2}^{222} - C_{-1,2,1}^{222})g_6 \Big\} .$$

Using the Clebsch-Gordon coefficients

$$C^{222}_{o,\pm 1,\pm 1} = - \sqrt{\frac{1}{14}}$$

$$C^{222}_{o,\pm 2,\pm 2} = \sqrt{\frac{2}{7}}$$

$$C^{222}_{\pm 1,\mp 2,\mp 1} = C^{222}_{\pm 2,\mp 1,\pm 1} = - C^{222}_{\pm 1,\pm 1,\pm 2} = \sqrt{\frac{3}{7}} \quad ,$$

we get

$$(\Psi^2_{2+'}, r^2_4 \, Y^{oo}_{2+}(\Gamma_4) \, \Psi^2_{2+'}) = \frac{a^2}{a^2_3} \frac{\sqrt{2}}{7} \left[\frac{\sqrt{2}}{3} (\frac{1}{2} g_1 + g_2) + \frac{1}{\sqrt{3}} (g_3 + g_4) - (g_5 + g_6) \right]$$

Putting in the value of Γ'_4 (suppressing the argument Γ'_4)

$$Y^{1o}_{2+}(+,-) \; Y^{-1,o}_{2+} = 0, \frac{2}{\sqrt{3}}$$

$$Y^{2o}_{2+}(+,-) \; Y^{-2,o}_{2+} = \frac{1}{\sqrt{6}} , 0$$

$$Y^{o,\pm 1}_{2+} = \mp \frac{1}{\sqrt{3}} e^{\pm 3\pi i/4}$$

$$Y^{o,\pm 2}_{2+} = \mp \frac{i}{\sqrt{6}}$$

$$Y^{1,\pm 1}_{2+}(+,-) \; Y^{-1,\pm 1}_{2+} = (\frac{1}{\sqrt{3}} , \mp \frac{1}{3}) \, e^{\pm 3\pi i/4}$$

$$Y^{1,\pm 2}_{2+}(+,-) \; Y^{-1,\pm 2}_{2+} = (i \frac{\sqrt{6}}{3} , \pm i \frac{\sqrt{2}}{3})$$

$$Y^{2,\pm 1}_{2+}(+,-) \; Y^{-2,\pm 1}_{2+} = (\pm \frac{\sqrt{2}}{3} , \frac{\sqrt{6}}{3}) \, e^{\pm 3\pi i/4}$$

$$Y^{2,\pm 2}_{2+}(+,-) \; Y^{-2,\pm 2}_{2+} = (\mp \frac{2i}{3} , \frac{-i}{\sqrt{3}})$$

we get

$$\frac{1}{2} g_1 + g_2 = 1$$

$$g_3 + g_4 = \frac{\sqrt{6}}{12}$$

$$g_5 + g_6 = 0 \quad .$$

$$Q'(q) = |a_2|^2 \cdot 16 \frac{ea^2}{\alpha_3^2} \cdot \frac{5}{42} = |a_2|^2 \cdot \frac{40}{21} \frac{ea^2}{\alpha_3^2}$$

$$= |a_2|^2 \cdot \frac{10}{21} \cdot \frac{937}{4.71} \text{ x e x } 1.11 \text{ x } 10^{-28} \text{ cm}^2 = |a_2|^2 \text{x } 1.05\text{e x } 10^{-26} \text{cm}^2$$

and on identification (a),

$$Q_a = (-2.7 + 13\ |a_2|^2)\text{e x } 10^{-27} \text{ cm}^2 \quad .$$

7. Comparison with Experiment.

Experimental data for the $\frac{1}{2}$ + → $\frac{5}{2}$ + transition rate in O^{17} and for the electric quadrupole moment and magnetic moment of the $\frac{5}{2}$ + ground state is summarized below.

		Reference
Transition	$4 \text{ x } 10^9 \text{ sec}^{-1}$	[16]
Quadrupole Moment	$(-5 \pm 2) \text{ e x } 10^{-27} \text{ cm}^2$	[17]
Magnetic Moment	$-1.8928 \pm 2\ \mu_o$	[18]

The calculated values for the transition rate are:

$1.6|a_ob_2 + \sqrt{3}\ b_oa_2^*|^2 \text{ x } 10^{10} \text{ sec}^{-1}$ on identification (b)

$1.2|a_ob_2 + \sqrt{3}\ b_oa_2^*|^2 \text{ x } 10^{9} \text{ sec}^{-1}$ on identification (a).

On identification (b), the observed rate is achieved with $|a_ob_2 + \sqrt{3}\ b_oa_2^*| = 0.5$. Given the most favorable phase relationship, $b_2 = a_2^*$, a quite low amplitude of core excitation, $|a_2| = |b_2| \sim 0.2$ (4 per cent probability of core excitation) is possible. On identification (a), no exact fit is possible. Taking $a_o = b_2 = 0$, $a_2 = b_o = 1$, for example, gives a rate of $3.6 \text{ x } 10^{10} \text{ sec}^{-1}$, which is in agreement with the experimental value; however $a_2 = 1$, corresponding to a completely excited core in the ground state, is not to be believed.

The computed values of the quadrupole moment

$(-2.7 + 18|a_2|^2)e \times 10^{-27}$ cm^2 on identification (b)

$(-2.7 + 13|a_2|^2)e \times 10^{-27}$ cm^2 on identification (a)

can never agree precisely with the observed value. On identification (b), with $|a_2| = 0.2$, $Q = -2e \times 10^{-27}$ cm^2 and the fit is fair; on identification (a), however, with a large value of $|a_2|$, the wrong sign of the quadrupole moment would be obtained.

The computed magnetic moment,

$$(-1.847 + .934|a_2|^2)\mu_0$$

likewise can never agree precisely with the experimental value. Here again identification (b), with $|a_2| = 0.2$, gives a value, $-1.81\mu_0$, which is in fair agreement; but identification (a) with a large value of $|a_2|$ produces no agreement. (It is to be noted however, that no model of 0^{17} based upon an orbital neutron and core can correctly predict the magnetic moment.)

Calculations of these data using more complicated wave functions, e.g., including $d_{3/2}$ neutron states, could be performed. However, it is expected that no improvement in the fit with experimental data would result.

PART V. SUMMARY

The excitation energies of states of O^{16}, computed on the α-particle model on either of the two identification schemes proposed by Dennison, are in quite good agreement with the observed energies. There are on either scheme several levels which are predicted but not observed; however, since the actual O^{16} nucleus contains a greater degree of symmetry than that which the α-particle model represents, this discrepancy is not serious. On identification (a), several of the observed levels are not predicted. However, if four of the energy levels above 12.5 Mev have $T = 1$, as predicted by the theory of equivalence between neutrons and protons, this evidence favors identification (a) over identification (b).

The lifetimes of the four lowest excited states have also been computed on this model. Here the agreement is only fair. The calculated 0^+ lifetime is too short by a factor of fifteen, while that of the 3^- state is too long by a factor of three or more. On identification (a), the calculated lifetime of the 2^+ state (and indirectly that of the 1^- state based upon the 2^+ lifetime) is definitely too long by a factor of greater than ten. On identification (b), the calculated lifetime of the 2^+ state agrees with the present experimental data; but if the experimental data should be improved, this apparent agreement may be removed.

Calculations on O^{17} have been performed, using the shell model with a neutron outside an O^{16} core and allowing for a partial 2^+ excitation of the core. If identification (a) is used to describe the 2^+ core state, the lifetime of the 870 Kev $\frac{1}{2}+$ state in O^{17} cannot be fitted. If identification (b) is used, the observed lifetime can be fitted, requiring only a 4 per cent probability of core excitation in both the $\frac{1}{2}$ + and $\frac{5}{2}$ + states. The calculated magnetic and electric quadrupole moments of the ground state are slightly too small in magnitude. However, as no model of O^{17} which treats of an orbital neutron and core can accurately match these moments, this discrepancy cannot be regarded as decreasing the validity of the α-particle model.

We conclude, therefore that the α-particle model predicts the energy levels of O^{16} rather well, but gives only fair agreement with the lifetimes of the lower excited states. Using the α-particle model to supply core wave functions for an excited core shell model of O^{17} can provide agreement with the observed lifetime of the 870 Kev $\frac{1}{2}$ + state, but cannot provide quantitative agreement with the electric quadrupole and magnetic moments of the ground state.

Since the energy level data tend to favor identification (a) while lifetime calculations favor identification (b), we do not find conclusive evidence for eliminating either of the two identification schemes proposed by Dennison.

APPENDIX I

GENERALIZED SPHERICAL HARMONICS (SYMMETRIC TOP WAVE FUNCTIONS)

The treatment reproduced here is almost exactly that given by Takehashi [5], except that the rotation operators S_x, S_y, S_z and S'_x, S'_y, S'_z are defined more in accordance with common usage, of half the magnitude of Takehashi's S operators. It is also hoped that the argument here is clearer.

Given an initial set of cartesian axes $\hat{i}'$, $\hat{j}'$, $\hat{k}'$ corresponding to coordinates x', y', z', we define a rotation of the coordinate axes through Euler angles ϕ, θ, Ψ into a final set of axes $\hat{i}$, $\hat{j}$, $\hat{k}$ to consist of first a rotation through angle ϕ about $\hat{k}'$

$$\hat{i}', \hat{j}', \hat{k}' \longrightarrow \hat{i}_{(1)}, \hat{j}_{(1)}, \hat{k}_{(1)}$$

$$\begin{pmatrix} \hat{i}_{(1)} \\ \hat{j}_{(1)} \\ \hat{k}_{(1)} \end{pmatrix} = R_z(\phi) \begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix} , \quad R_z(\phi) \equiv \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

followed by a rotation through θ about $\hat{j}_{(1)}$ (the transformed $\hat{j}'$ axis),

$$\hat{i}'_{(1)}, \hat{j}'_{(1)}, \hat{k}'_{(1)} \longrightarrow \hat{i}_{(2)}, \hat{j}_{(2)}, \hat{k}_{(2)}$$

$$\begin{pmatrix} \hat{i}_{(2)} \\ \hat{j}_{(2)} \\ \hat{k}_{(2)} \end{pmatrix} = R_y(\theta) \begin{pmatrix} \hat{i}_{(1)} \\ \hat{j}_{(1)} \\ \hat{k}_{(1)} \end{pmatrix} = R_y(\theta)\, R_z(\phi) \begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix} ;$$

$$R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}$$

followed lastly by a rotation through Ψ about $\hat{k}_{(2)}$ (the transformed $\hat{k}'$ axis):

$$\hat{i}_{(2)},\ \hat{j}_{(2)},\ \hat{k}_{(2)} \longrightarrow \hat{i},\ \hat{j},\ \hat{k}$$

$$\begin{pmatrix} \hat{i} \\ \hat{j} \\ \hat{k} \end{pmatrix} = R_z(\Psi) \begin{pmatrix} \hat{i}_{(2)} \\ \hat{j}_{(2)} \\ \hat{k}_{(2)} \end{pmatrix} = R_z(\Psi)\ R_y(\theta)\ R_z(\phi) \begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix}$$

$$\equiv R(\phi, \theta, \Psi) \begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix}$$

where by definition $R(\phi, \theta, \Psi) = R_z(\Psi)\ R_y(\theta)\ R_z(\phi)$. We have adopted the convention that the rotation through Ψ, θ, ϕ is merely a change of reference coordinates. Hence in the rotation, a position vector $x'\hat{i}' + y'\hat{j}' + z'\hat{k}' = x\hat{i} + y\hat{j} + z\hat{k}$ remains invariant. Thus the coordinates x', y', z' undergo a transformation which is the inverse of the transformation of the coordinate axes:

$$x', y', z' \longrightarrow x, y, z\ , \quad \text{where}$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = R^{-1}(\phi, \theta, \Psi) \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R_z(-\Psi)\ R_y(-\theta)\ R_z(-\Psi) \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} \qquad (2)$$

The rotations through angles ϕ, θ, Ψ form a group, and the matrices $R(\phi, \theta, \Psi)$ a three dimensional representation of that group with basis $\hat{i}', \hat{j}', \hat{k}'$ (or x, y, z). *However we desire to find* explicitly the most general representation D^J_{km} of dimension $2J + 1$ of the rotation group and the basis vectors Y^{km}_J of the representation.

To do this we fix attention on the coordinates x, y, z of a point on the unit sphere, and establish the homomorphism

$$\xi\ ,\eta \ \text{-->}\ x,\ y,\ z \qquad \text{with}$$

$$\begin{aligned} x + iy &= 2\,\eta\,\bar{\xi} \\ x - iy &= 2\,\xi\,\bar{\eta} \\ z &= \xi\bar{\xi} - \eta\bar{\eta} \end{aligned} \tag{3}$$

$$\sqrt{x^2 + y^2 + z^2} = \xi\bar{\xi} + \eta\,\bar{\eta} = 1$$

If we regard x, y, z as transformed coordinates of a point x_o, y_o, z_o then by eq. (2):

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = R_z(-\phi)\ R_y(-\theta)\ R_z(-\Psi) \begin{pmatrix} x_o \\ y_o \\ z_o \end{pmatrix}$$

which may be paralleled by

$$\begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} e^{\frac{-i\phi}{2}} & 0 \\ 0 & e^{\frac{i\phi}{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} e^{\frac{-i\Psi}{2}} & 0 \\ 0 & e^{\frac{i\Psi}{2}} \end{pmatrix} \begin{pmatrix} \xi_o \\ \eta_o \end{pmatrix}$$

or

$$\begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} e^{\frac{-i}{2}(\phi+\Psi)} \cos\frac{\theta}{2} & -e^{\frac{-1}{2}(\phi-\Psi)} \sin\frac{\theta}{2} \\ e^{\frac{i}{2}(\phi-\Psi)} \sin\frac{\theta}{2} & e^{\frac{i}{2}(\phi+\Psi)} \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \xi_o \\ \eta_o \end{pmatrix} \tag{4}$$

If we use a bar to indicate complex conjugate, we may also write

$$\begin{pmatrix} \xi & -\bar{\eta} \\ \eta & \bar{\xi} \end{pmatrix} = \begin{pmatrix} e^{\frac{-i}{2}(\phi+\Psi)} \cos\frac{\theta}{2} & -e^{\frac{-i}{2}(\phi-\Psi)} \sin\frac{\theta}{2} \\ e^{\frac{i}{2}(\phi-\Psi)} \sin\frac{\theta}{2} & e^{\frac{i}{2}(\phi+\Psi)} \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \xi_o & -\bar{\eta}_o \\ \eta_o & \bar{\xi}_o \end{pmatrix} \tag{4'}$$

If we identify $\xi_o = 1$, $\eta_o = 0$, and in general take

$$\xi = e^{\frac{-i}{2}(\phi+\Psi)} \cos \frac{\theta}{2}$$

$$\eta = e^{\frac{i}{2}(\phi-\Psi)} \sin \frac{\theta}{2}$$

we see that the matrices $\begin{pmatrix} \xi & -\bar{\eta} \\ \eta & \bar{\xi} \end{pmatrix}$ form a group under rotations and if $\begin{pmatrix} \xi & -\bar{\eta} \\ \eta & \bar{\xi} \end{pmatrix}$ represent the rotation which transforms x_1, y_1, z_1 into x_2, y_2, z_2, then

$$\begin{pmatrix} \xi_2 & -\bar{\eta}_2 \\ \eta_2 & \bar{\xi}_2 \end{pmatrix} = \begin{pmatrix} \xi & -\bar{\eta} \\ \eta & \bar{\xi} \end{pmatrix} \begin{pmatrix} \xi_1 & -\bar{\eta}_1 \\ \eta_1 & \bar{\xi}_1 \end{pmatrix} \qquad (4'')$$

We shall at this point switch to the adjoint of these equations and use right hand group multiplication which turns out to be a bit more convenient and agrees with Takehashi's usage.

$$\begin{pmatrix} \bar{\xi}_2 & \bar{\eta}_2 \\ -\bar{\eta}_2 & \xi_2 \end{pmatrix} = \begin{pmatrix} \bar{\xi}_1 & \bar{\eta}_1 \\ -\bar{\eta}_1 & \xi_1 \end{pmatrix} \begin{pmatrix} \bar{\xi} & \bar{\eta} \\ -\eta & \xi \end{pmatrix} \qquad (5)$$

and we may denote

$$\Gamma_i = \begin{pmatrix} \bar{\xi}_i & \bar{\eta}_i \\ -\eta_i & \xi_i \end{pmatrix}, \qquad \Gamma = \begin{pmatrix} e^{\frac{i}{2}(\phi+\Psi)} \cos \frac{\theta}{2} & e^{\frac{-i}{2}(\phi-\Psi)} \sin \frac{\theta}{2} \\ -e^{\frac{-i}{2}(\phi-\Psi)} \sin \frac{\theta}{2} & e^{\frac{-i}{2}(\phi+\Psi)} \cos \frac{\theta}{2} \end{pmatrix} \qquad (6)$$

then

$$\Gamma_1 \to \Gamma_2 \quad \text{is denoted by} \quad \Gamma_2 = \Gamma_1 \, \Gamma \qquad (5')$$

and Γ forms a right handed two-valued representation of the rotation group with basis $\overparen{\underparen{\bar{\xi}\ \ \bar{\eta}}}$ or $\overparen{\underparen{-\eta\ \ \xi}}$.

Spherical harmonics of order J may be generated by

$$\frac{1}{J!}\left(-\frac{1}{2}(x+iy)p^2+zpq+\frac{1}{2}(x-iy)q^2\right)^J=\sum_{m=-J}^{J}Y_J^m\frac{p^{J+m}q^{J-m}}{\sqrt{(J+m)!(J-m)!}}\tag{7}$$

since it can easily be shown that Y_J^m are homogeneous functions of order J in x, y, z which satisfy Laplace's equation.

This could be written more simply

$$\frac{(\bar{\xi}p+\bar{\eta}q)^J(-\eta p+\xi q)^J}{J!}=\sum_{m=-J}^{J}Y_J^m\frac{p^{J+m}q^{J-m}}{\sqrt{(J+m)!\ (J-m)!}}\tag{7'}$$

We obtain the generalized spherical harmonics Y_J^{km} $(|k|,\ |m|\leq J)$ from the expansion

$$\frac{(\bar{\xi}p+\bar{\eta}q)^{J+k}(-\eta p+\xi q)^{J-k}}{\sqrt{(J+k)!\ (J-k)!}}=\sum_{m=-J}^{J}Y_J^{km}\frac{p^{J+m}q^{J-m}}{\sqrt{(J+m)!\ (J-m)!}}\tag{8}$$

in which J, k, m, may be simultaneously integers or half integers.

If we define the spinor $\mathbb{P}$ and the function $U_J^k(\mathbb{P})$ as

$$\mathbb{P}=\begin{pmatrix}p\\q\end{pmatrix};\qquad U_J^k(\mathbb{P})=\frac{p^{J+k}q^{J-k}}{\sqrt{(J+k)!\ (J-k)!}}\ .\tag{9}$$

Then equation (9) may be written

$$U_J^k(\Gamma\mathbb{P})=\sum_m Y_J^{km}(\Gamma)\ U_J^m(\mathbb{P})\tag{10}$$

or as shorthand

$$U_J(\Gamma\mathbb{P})=Y_J(\Gamma)\ U_J(\mathbb{P})\tag{10'}$$

where it is understood that $U_J(\mathbb{P})$ is a column vector of $2J + 1$ elements, and $Y_J(\Gamma)$ is a square matrix of order $2J + 1$ with c umns k and rows m. We also see that

$$Y_{\frac{1}{2}}(\Gamma) = \Gamma \quad .$$

Applying eq. (5) we get

$$U_J(\Gamma_2 \mathbb{P}) = U_J(\Gamma_1 \, \Gamma \mathbb{P}) = Y_J(\Gamma_1) \, U_J(\Gamma \mathbb{P}) = Y_J(\Gamma_1) \, Y_J(\Gamma) \, U_J(\mathbb{P})$$

whence

$$Y_J(\Gamma_2) = Y_J(\Gamma_1) \, Y_J(\Gamma)$$

or

$$Y_J^{km}(\Gamma_2) = \sum_h Y_J^{kh}(\Gamma_1) \, Y_J^{hm}(\Gamma) \quad . \tag{11}$$

Thus for fixed k, Y_J^{km}, $- J \leq m \leq J$ form the basis for a $2J + 1$-dimension row representation D_J, and at the same time Y_J^{km} forms a right-handed representation of the group.

If we write iS_x, iS_y, iS_z as right-handed operators on Γ corresponding to infinitesimal rotations about the final $\hat{i}, \hat{j}, \hat{k}$ axes, we have

$$S_x = - i \left.\frac{\partial\Gamma}{\partial\theta}\right|_{-\frac{\pi}{2}, \, 0, \, \frac{\pi}{2}} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = - i \left.\frac{\partial\Gamma}{\partial\theta}\right|_{0,0,0} = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$S_z = - i \left.\frac{\partial\Gamma}{\partial\phi}\right|_{0,0,0} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12}$$

If we call

$$S_+ = S_x + iS_y = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad S_- = S_x - iS_y = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{13}$$

$$S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{1}{2}(S_+ S_- + S_- S_+) + S_z^2$$

and consider using these operators as left hand operators on ,

then formally

$$S_+ \mathbb{P} = \begin{pmatrix} q \\ 0 \end{pmatrix} = q \frac{\partial}{\partial p} \mathbb{P}$$

$$S_- \mathbb{P} = \begin{pmatrix} 0 \\ p \end{pmatrix} = p \frac{\partial}{\partial q} \mathbb{P}$$

$$S_z \mathbb{P} = \frac{1}{2} \begin{pmatrix} p \\ -q \end{pmatrix} = \frac{1}{2} (p \frac{\partial}{\partial p} - q \frac{\partial}{\partial q}) \mathbb{P} \quad .$$

Hence if we define the scalar product of two spinors

$$(\mathbb{P}', \mathbb{P}) = \bar{p}', p + \bar{q}' q = (\bar{p}', \bar{q}') \begin{pmatrix} p \\ q \end{pmatrix} = \tilde{\mathbb{P}}' \mathbb{P} \qquad (13')$$

(~ denotes Hermitian adjoint)

and we note that

$$q \frac{\partial}{\partial p} (\mathbb{P}', \Gamma \mathbb{P}) = (\mathbb{P}', \Gamma(S_+ \mathbb{P})) = (\mathbb{P}', (\Gamma S_+) \mathbb{P}) \equiv S_+(\mathbb{P}', \Gamma \mathbb{P}) \qquad (14)$$

and if regard S_+, S_-, S_z written outside and the left as operators on the quantity to the right of the comma, it makes no difference whether we regard S as operating to the right on Γ or to the left on $\mathbb{P}$.

Now if we consider the definition of $U_J(\mathbb{P})$ from eq. (9), together with the definition of $U_J(\Gamma)$ from eq. (10'), we find

$$\frac{1}{(2J)!} (\mathbb{P}', \Gamma \mathbb{P})^{2J} = (U_J(\mathbb{P}'), U_J(\Gamma \mathbb{P})) = (U_J(\mathbb{P}), Y_J(\Gamma)\, U_J(\mathbb{P}))$$

$$= \sum_{k=-J}^{J} \sum_{m=-J}^{J} Y_J^{km}(\Gamma)\, U_J^m(\mathbb{P})\, U_J^k(\bar{\mathbb{P}}') \qquad (15)$$

and if we define

$$S\, Y_J^{km}(\Gamma) \equiv Y_J^{km}(\Gamma\, S)$$

and noting that

$$\begin{aligned} q\,\frac{\partial}{\partial p}\,U_J^{m'}(\mathbb{P}) &= \sqrt{(J+m')(J-m'+1)}\;U_J^{m'-1}(\mathbb{P}) \\ p\,\frac{\partial}{\partial q}\,U_J^{m'}(\mathbb{P}) &= \sqrt{(J-m)(J+m+1)}\;U_J^{m'+1}(\mathbb{P}) \\ \frac{1}{2}\left(p\,\frac{\partial}{\partial p} - q\,\frac{\partial}{\partial q}\right)U_J^{m'}(\mathbb{P}) &= m'\,U_J^{m'}(\mathbb{P}) \quad , \end{aligned} \tag{16}$$

we apply operators S to eq. (15) and equate expressions with S operating on Γ to those with S operating on $\mathbb{P}$, we get:

$$\begin{aligned} S_+\,Y_J^{km}(\Gamma) &= \sqrt{(J-m)(J+m+1)}\;Y_J^{k,m+1}(\Gamma) \\ S_-\,Y_J^{km}(\Gamma) &= \sqrt{(J+m)(J-m+1)}\;Y_J^{k,m-1}(\Gamma) \\ S_z\,Y_J^{km}(\Gamma) &= m\,Y_J^{km}(\Gamma) \\ S^2\,Y_J^{km}(\Gamma) &= J(J+1)\,Y_J^{km}(\Gamma) \quad . \end{aligned} \tag{17}$$

To consider infinitesimal rotations about the initial $\hat{i}', \hat{j}', \hat{k}'$ axes, note that for any rotation S about $\hat{i}, \hat{j}, \hat{k}$, the corresponding rotation S' about $\hat{i}', \hat{j}', \hat{k}'$ can be performed by undoing the rotation Γ, performing S, and then rotating through Γ:

$$S' = \Gamma^{-1}\, S\, \Gamma$$

or (18)

$$\Gamma\, S' = S\, \Gamma$$

Therefore $S'(\mathbb{P}', \Gamma\mathbb{P}) = (\mathbb{P}', S\,\Gamma\mathbb{P}) = (\tilde{S}\,\mathbb{P}', \Gamma\mathbb{P})$, where $\tilde{S}$ is the Hermitian adjoint of S; but

$$\tilde{S}_+ = S_- , \qquad \tilde{S}_- = S_+ , \qquad \tilde{S}_z = S_z$$

and by the symmetry of eq. (15) with respect to $\mathbb{P}$ and $\mathbb{P}'$, k and m, we get:

$$S'_+ \, Y_J^{km}(\Gamma) = \sqrt{(J+k)(J-k+1)} \; Y_J^{k-1,m}(\Gamma)$$

$$S'_- \, Y_J^{km}(\Gamma) = \sqrt{(J-k)(J+k+1)} \; Y_J^{k+1,m}(\Gamma)$$

$$S'_z \, Y_J^{km}(\Gamma) = k \, Y_J^{km}(\Gamma) \tag{19}$$

$$S'^2 = S^2$$

$$S'^2 \, Y_J^{km}(\Gamma) = J(J+1) \, Y_J^{km}(\Gamma) \quad .$$

We can now demonstrate that $Y_J^{km}(\Gamma)$ are symmetric top wave functions. The Hamiltonian for a symmetric top is given by:

$$H = a(M'^2_x + M'^2_y) + cM'^2_z \qquad \text{where} \quad M'_{x,y,z} = \hbar \, S'_{x,y,z}$$

$$= \hbar^2 (aS^2 + (c-a) \, S'^2_z) \quad .$$

Thus

$$H \, Y_J^{km}(\Gamma) = \hbar^2 [aJ(J+1) + (c-a)k^2] \; Y_J^{km}(\Gamma) \quad ,$$

showing that Y_J^{km} are eigenfunctions for the symmetric top wave equation, with energy $\hbar^2[aJ(J+1) + (c-a)k^2]$.

Explicit Expressions, Normalization, and Special Properties of $Y_J^{km}(\Gamma)$.

Performing the expansion indicated in eq. (15):

$$\frac{1}{(2J)!} (\mathcal{P}', \Gamma \mathcal{P})^{2J} = \sum_{km} Y_J^{km}(\Gamma) \, U_J^m(\mathcal{P}) \, U_J^k(\mathcal{P}')$$

$$= \sum_k \frac{(\bar{\xi} \, p + \bar{\eta} \, q)^{J+k} \, (-\eta \, p + \xi \, q)^{J-k}}{\sqrt{(J+k)! \, (J-k)!}} \, U_J^k(\bar{\mathcal{P}}')$$

$$= \sum_{mk} U_J^m(\mathcal{P}) \, U_J^k(\bar{\mathcal{P}}') \sum_v \frac{\sqrt{(J+m)! \, (J-m)! \, (J+k)! \, (J-k)!}}{(J+m-v)! \, (J-k-v)! \, (k-m+v)! \, v!}$$

$$\times \, (\bar{\xi})^{J+m-v} \; \xi^{J-k-v} \; (\bar{\eta})^{k-m+v} (-\eta)^v$$

hence

$$Y_J^{km}(\Gamma) = \sum_v (-1)^v \frac{\sqrt{(J+m)!\ (J-m)!\ (J+k)!\ (J-k)!}}{(J+m-v)!\ (J-k-v)!\ (k-m+v)!\ v!}$$

$$\times\ \bar{\xi}^{\,J+m-v}\ \xi^{J-k-v}\ \bar{\eta}^{\,k-m+v}\ \eta^{v} \tag{20}$$

$$= e^{i(m\phi+k\Psi)}\ P_J^{km}(\theta) \tag{21}$$

where the generalized Legendre function $P_J^{km}(\theta)$ is equal to:

$$P_J^{km}(\theta) = \sum_v (-1)^v \frac{\sqrt{(J+m)!\ (J-m)!\ (J+k)!\ (J-k)!}}{(J+m-v)!\ (J-k-v)!\ (k-m+v)!\ v!}$$

$$\times\ (\cos\frac{\theta}{2})^{2J+m-k-2v}\ (\sin\frac{\theta}{2})^{k-m+2v}\ . \tag{21'}$$

From eq. (11) we then have for $\Gamma_2 = \Gamma_1\ \Gamma$

$$P_J^{km}(\theta_2)\ e^{i(k\Psi_2+M\phi_2)} = \sum_{h=-J}^{J} P_J^{kh}(\theta_1)\ P_J^{hm}(\theta)\ e^{i(k\Psi_1+h[\phi_1+\Psi]+m\phi)} . \tag{22}$$

If we define

$$\Theta = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \tag{23}$$

$$P_J^{km}(\theta) = Y_J^{km}(\Theta) \tag{24}$$

for the special cases

$$\Gamma_a = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \qquad \eta = \bar{\eta} = 0 \tag{25}$$

$$\Gamma_b = \begin{pmatrix} 0 & c \\ d & 0 \end{pmatrix} \qquad \xi = \bar{\xi} = 0 \ .$$

$$Y_J^{km}(\Gamma_a) = a^{J+m}\ b^{J-m}\ \delta_{km}\ , \qquad Y_J^{km}(\Gamma_b) = c^{J+k}\ d^{J-k}\delta_{k,-m} \tag{26}$$

From which we derive the properties of $P_J^{km}(\theta)$:

$$P_J^{km}(\theta + \theta') = \sum_{h=-J}^{J} P_J^{kh}(\theta)\, P_J^{hm}(\theta') \tag{22'}$$

$$P_J^{km}(\theta) = \delta_{k,m} \qquad P_J^{km}(\pm \pi) = (-1)^{J \mp k}\, \delta_{k,-m} \tag{27}$$

$$P_J^{km}(2\pi) = (-1)^{2J}\, \delta_{k,m} \qquad P_J^{km}(\theta \pm \pi) = (-1)^{J \mp k}\, P_J^{-k,m}(\theta)\ . \tag{28}$$

By applying the formal relation

$$\Theta_{-\theta} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} (\Theta_\theta) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{29}$$

with

$$Y_J^{km} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = (-1)^{J-k}\, \delta_{k,m}$$

$$P_J^{km}(-\theta) = \sum_{hl} Y_J^{kh} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} P_J^{hl}(\theta)\, Y_J^{lm} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = (-1)^{m-k}\, P_J^{km}(\theta) \tag{30}$$

$$= P_J^{mk}(\theta) = P_J^{-k,-m}(\theta) \quad ;$$

and by the formal relation

$$\Theta = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \Theta_{\pi/2} \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix} \Theta_{-\pi/2} \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \tag{31}$$

we get

$$P_J^{km}(\theta) = \sum_h i^{(-J+k)}\, P_J^{kh}(\tfrac{\pi}{2})\, e^{ih\theta}\, P_J^{hm}(-\tfrac{\pi}{2})\, i^{(J-m)}$$

$$= \sum_h i^{(k-m)}\, e^{ih\theta}\, P_J^{kh}(\tfrac{\pi}{2})\, P_J^{km}(-\tfrac{\pi}{2}) \tag{32}$$

Then using

$$P_J^{k,-h}(\tfrac{\pi}{2}) = P_J^{-k,h}(-\tfrac{\pi}{2}) = (-1)^{J+k}\, P_J^{kh}(\tfrac{\pi}{2}) \qquad (30')$$

$$P_J^{k,-h}(\tfrac{\pi}{2})\, P_J^{m,-h}(\tfrac{\pi}{2}) = (-1)^{k-m}\, P_J^{kh}(\tfrac{\pi}{2})\, P_J^{mh}(\tfrac{\pi}{2}) \quad ,$$

we get

$$P_J^{km}(\theta) = (-1)^{\frac{k-m}{2}} \quad P_J^{ko}(\tfrac{\pi}{2})\, P_J^{mo}(\tfrac{\pi}{2}) + \sum_{h>o} \cos(h\theta+(k-m)\,\tfrac{\pi}{2})\, P_J^{kh}(\tfrac{\pi}{2})\, P_J^{mh}(\tfrac{\pi}{2}) \qquad (33)$$

To obtain a more convenient expression for $P_J^{km}(\theta)$, observe that for $\Psi = \emptyset = 0$, $\Gamma = \Theta$

$$U_J^k(\Theta\, \mathbb{P}) = \sum_{m=-J}^{J} P_J^{km}(\theta)\, \frac{p^{J+m}\, q^{J-m}}{\sqrt{(J+m)!\ (J-m)!}} \qquad (34)$$

hence

$$P_J^{km}(\theta) = \sqrt{\frac{(J-m)!}{(J+m)!}}\ \left\{ (\frac{d}{dp})^{J+m}\, U_J^k(\Theta\, \mathbb{P}) \right\}_{p=o,q=1} \qquad (35)$$

$$= \sqrt{\frac{(J+m)!}{(J-m)!}}\ \left\{ (\frac{d}{dq})^{J-m}\, U_J^k(\Theta\, \mathbb{P}) \right\}_{p=1,q=o} \quad .$$

But

$$U_J^k(\Theta\, \mathbb{P}) = (p \cos \frac{\theta}{2} + q \sin \frac{\theta}{2})^{J+k}\ (-p \sin \frac{\theta}{2} + q \cos \frac{\theta}{2})^{J-k} \ ; \qquad (36)$$

hence if we let $q = 1$ and $t = \cos\theta - p \sin\theta$

$$1 - t = (1 - \cos\theta) + p \sin\theta = 2 \sin \frac{\theta}{2}\ (\sin \frac{\theta}{2} + p \cos \frac{\theta}{2})$$

$$1 + t = (1 + \cos\theta) + p \sin\theta = 2 \cos \frac{\theta}{2}\ (\cos \frac{\theta}{2} - p \sin \frac{\theta}{2})$$

$$U_J^k(\Theta\, \mathbb{P})_{q=1} = \frac{(1 - t)^{J+k}\ (1 - t)^{J-k}}{2^{2J}\ \sin^{J+k} \frac{\theta}{2} \cos^{J-k} \frac{\theta}{2}\ \sqrt{(J-k)!\ (J+k)!}} \qquad (37)$$

$$\left.\frac{d}{dp}\right|_{\substack{p=o\\ q=1}} = - \sin \theta \frac{d}{dt} ,$$

$$\left.\left(\frac{d}{dp}\right)^{J+m}\right|_{\substack{p=o\\ q=1}} = (-1)^{J+m} \, 2^{J+m} \sin^{J+m} \frac{\theta}{2} \cos^{J+m} \frac{\theta}{2} \left.\left(\frac{d}{dt}\right)^{J+m}\right|_{\substack{p=o\\ q=1}}$$

hence

$$P_J^{km}(\theta) = \frac{(-1)^{m-k}}{2^{J-m}} \sqrt{\frac{(J-m)!}{(J+m)!\,(J-k)!\,(J+k)!}} \sin^{m-k} \frac{\theta}{2} \cos^{m+k} \frac{\theta}{2}$$

$$\times \left(\frac{d}{d[\cos \theta]}\right)^{J+m} [(\cos \theta + 1)^{J-k} (\cos \theta + 1)^{J+k}] \qquad (38)$$

If we write $z = \cos \theta$, $\sin \frac{\theta}{2} = 2^{-1/2} (1 - z)^{1/2}$; $\cos \frac{\theta}{2} = 2^{-1/2}(1 + z)^{1/2}$

$$P_J^{km}(z) = (-1)^{m-k} \, 2^{-J} \sqrt{\frac{(J-m)!}{(J+m)!\,(J-k)!\,(J+k)!}} (1-z)^{\frac{m-k}{2}} (1+z)^{\frac{m+k}{2}}$$

$$\times \left(\frac{d}{dz}\right)^{J+m} [(z + 1)^{J-k} (z - 1)^{J+k}] \qquad (39)$$

Applying eq. (32), we get alternate expressions

$$P_J^{km}(z) = 2^{-J} \sqrt{\frac{(J-k)!}{(J+k)!\,(J-m)!\,(J+m)!}} (1-z)^{\frac{k-m}{2}} (1+z)^{\frac{k+m}{2}}$$

$$\times \left(\frac{d}{dz}\right)^{J+k} [(z + 1)^{J-m} (z - 1)^{J+m}] \qquad (40)$$

$$= 2^{-J} \sqrt{\frac{(J+m)!}{(J-m)!\,(J+k)!\,(J-k)!}} (1-z)^{\frac{k-m}{2}} (1+z)^{\frac{-m-k}{2}}$$

$$\times \left(\frac{d}{dz}\right)^{J-m} [(z + 1)^{J+k} (z - 1)^{J-k}] \qquad (41)$$

$$= (-1)^{m-k} \sqrt{\frac{(J+k)!}{(J-k)!\,(J-m)!\,(J+m)!}} (1-z)^{\frac{m-k}{2}} (1+z)^{\frac{-m-k}{2}}$$

$$\times \left(\frac{d}{dz}\right)^{J-k} [(z + 1)^{J+m} (z - 1)^{J-m}] \qquad (42)$$

Orthogonality

$$\int_{-1}^{1} P_J^{km}(z)\, P_{J'}^{km}(z)\, dz = \frac{2}{2J + 1}\, \delta_{J,J'} \qquad (43)$$

$$\int_0^{\pi} \int_0^{2\pi} \int_0^{2\pi} Y_J^{km}\, \overline{Y}_{J'}^{k',m'} \sin\theta\, d\Psi\, d\phi\, d\theta = \frac{8\pi^2}{2J + 1}\, \delta_{JJ'}\, \delta_{mm'}\, \delta_{kk'}$$

(44)

APPENDIX II

TABLE OF GENERALIZED LEGENDRE FUNCTIONS $P_J^{km}(\theta)$; $0 \leq J \leq 4$.

The listed functions have $m \geq k \geq 0$. All others can be found from the relations of eq. AI.28 and AI.30.

$$\begin{aligned} P_J^{km}(\theta) &= P_J^{-m,-k}(\theta) = (-1)^{k-m}\, P_J^{-k,-m}(\theta) = (-1)^{k-m}\, P_J^{m,k}(\theta) \\ &= (-1)^{J\pm k}\, P_J^{-k,m}(\theta\pm\pi) = P_J^{m,k}(-\theta) = (-1)^{J-k}\, P_J^{k,-m}(\pi-\theta) \\ &= (-1)^{J-k}\, P_J^{m,-k}(\pi-\theta) = (-1)^{J+m}\, P_J^{-k,m}(\pi-\theta) = (-1)^{J+m}\, P_J^{-m,k}(\pi-\theta) \end{aligned}$$

$$P_o^{oo}(\theta) = 1$$

$$P_1^{11}(\theta) = \frac{1}{2}\,(1 + \cos\,\theta)$$

$$P_1^{o1}(\theta) = -\frac{1}{\sqrt{2}}\,\sin\,\theta$$

$$P_1^{oo}(\theta) = \cos\,\theta$$

$$P_2^{22}(\theta) = \frac{1}{4}\,(1 + \cos\,\theta)^2$$

$$P_2^{12}(\theta) = -\frac{1}{2}\,\sin\,\theta\,(1 + \cos\,\theta)$$

$$P_2^{o2}(\theta) = \frac{1}{4}\,\sqrt{6}\,\sin^2\,\theta$$

$$P_2^{11}(\theta) = \frac{1}{2}\,(2\,\cos\,\theta - 1)(1 + \cos\,\theta)$$

$$P_2^{o1}(\theta) = -\sqrt{\frac{3}{2}}\,\sin\,\theta\,\cos\,\theta$$

$$P_2^{oo}(\theta) = \frac{1}{2}\,(3\,\cos^2\,\theta - 1)$$

$$P_3^{33}(\theta) = \frac{1}{8}\,(1 + \cos\,\theta)^3$$

$$P_3^{23}(\theta) = -\frac{1}{8}\,\sqrt{6}\,\sin\,\theta\,(1 + \cos\,\theta)^2$$

$$P_3^{13}(\theta) = \frac{1}{8}\sqrt{15}\ \sin^2\theta\ (1 + \cos\theta)$$

$$P_3^{o3}(\theta) = -\frac{1}{4}\sqrt{5}\ \sin^3\theta$$

$$P_3^{22}(\theta) = \frac{1}{4}\ (-2 - \cos\theta + 4\cos^2\theta + 3\cos^3\theta)$$

$$P_3^{12}(\theta) = \frac{1}{8}\sqrt{10}\ [\,2\sin^3\theta - \sin\theta\ (1 + \cos\theta)^2\,]$$

$$P_3^{o2}(\theta) = \frac{1}{4}\sqrt{30}\ \sin^2\theta\cos\theta$$

$$P_3^{11}(\theta) = -\frac{1}{8}\ (1 + 11\cos\theta - 5\cos^2\theta + \cos^3\theta)$$

$$P_3^{o1}(\theta) = -\frac{1}{4}\sqrt{3}\ \sin\theta\ (5\cos^2\theta - 1)$$

$$P_3^{oo}(\theta) = \frac{1}{2}\cos\theta\ (5\cos^2\theta - 3)$$

$$P_4^{44}(\theta) = \frac{1}{16}\ (1 + \cos\theta)^4$$

$$P_4^{34}(\theta) = -\frac{1}{8}\sqrt{2}\ \sin\theta\ (1 + \cos\theta)^3$$

$$P_4^{24}(\theta) = \frac{1}{8}\sqrt{7}\ \sin^2\theta\ (1 + \cos\theta)^2$$

$$P_4^{14}(\theta) = -\frac{1}{8}\sqrt{14}\ \sin^3\theta\ (1 + \cos\theta)$$

$$P_4^{o4}(\theta) = \frac{1}{16}\sqrt{70}\ \sin^4\theta$$

$$P_4^{33}(\theta) = -\frac{1}{16}\ [\,7\sin^2\theta\ (1 + \cos\theta)^2 - (1 + \cos\theta)^4\,]$$

$$P_4^{23}(\theta) = \frac{1}{16}\sqrt{14}\ [\,3\sin^3\theta\ (1 + \cos\theta) - \sin\theta\ (1 + \cos\theta)^3\,]$$

$$P_4^{13}(\theta) = -\frac{1}{16}\sqrt{7}\,[\,5\sin^4\theta - 3\sin^2\theta\ (1 - \cos\theta)^2\,]$$

$$P_4^{o3}(\theta) = \frac{1}{4}\sqrt{35}\ \sin^3\theta\cos\theta$$

$$P_4^{22}(\theta) = \frac{1}{16}\ [\,15\sin^4\theta - 12\sin^2\theta\ (1 + \cos\theta)^2 + (1 + \cos\theta)^4\,]$$

$$P_4^{12}(\theta) = -\frac{1}{16}\sqrt{2}\ [\,10\sin^3\theta\ (1 - \cos\theta) - 15\sin^3\theta\ (1 + \cos\theta)$$
$$+\ 3\sin\theta\ (1 + \cos\theta)^3\,]$$

$$P_4^{o2}(\theta) = \frac{1}{16} \sqrt{10} \left[3 \sin^2 \theta \, (1 - \cos \theta)^2 - 8 \sin^4 \theta + 3 \sin^2 \theta (1 + \cos \theta)^2 \right]$$

$$P_4^{11}(\theta) = - \frac{1}{16} [10 \sin^2 \theta (1 - \cos \theta)^2 - 30 \sin^4 \theta$$

$$+ 15 \sin^2 \theta \, (1 + \cos \theta)^2 - (1 + \cos \theta)^4]$$

$$P_4^{o1}(\theta) = \frac{1}{8} \sqrt{5} \, [\sin \theta \, (1 - \cos \theta)^3 + 12 \sin^3 \theta \cos \theta$$

$$- \sin \theta \, (1 + \cos \theta)^3]$$

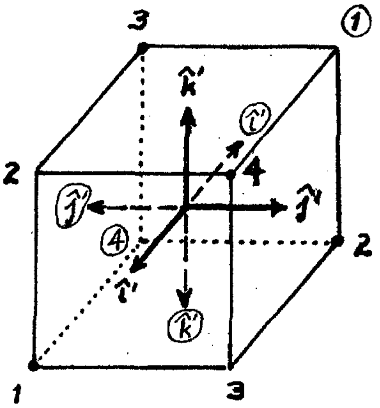
$$P_4^{oo}(\theta) = \frac{1}{8} (3 - 30 \cos^2 \theta + 35 \cos^4 \theta)$$

APPENDIX III

STANDARD ROTATIONAL REPRESENTATION OF PERMUTATION GROUP P.

Standard configuration 1,2,3,4
$\hat{i}'$, $\hat{j}'$, $\hat{k}'$ are a right-handed
system of axes.

Inverted configuration ①,②,③,④
$\textcircled{\hat{i}'}$, $\textcircled{\hat{j}'}$, $\textcircled{\hat{k}'}$ are a left-handed
system of axes.



The permutations of the group P are to be regarded as relabelling of coordinates. Thus in the equivalent rotation, the axes rotate but the particles are regarded as fixed in space. It is most convenient to regard the rotation in terms of fixed axes: ϕ, θ, Ψ is a rotation of Ψ about $\hat{k}'$, followed by θ about the original $\hat{j}'$, followed by ϕ about the original $\hat{k}'$.

The generators of the group P are the six elements of class (12) of simple permutations. Each of these involves a rotation through total angle π and an inversion which commutes with the rotation.

Any other element is formed by left-handed group multiplication, i.e.:

(12)(34) = (34)(12), but

(123) = (12)(23) = (23) followed by (12)

(1234) = (12)(23)(34) = (34) followed by (23) followed by (12) .

It follows that all odd elements (classes (12) and (1234)) are equivalent to a rotation and inversion which commutes with the rotation, and all even permutations (classes (12)(34) and (123)) are equivalent to a pure rotation.

The table on the following pages gives the rotation $\emptyset$, θ, Ψ and parity p (-1 for inversion), together with the three dimensional representation R_S

$$\begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix} \longrightarrow R_S \begin{pmatrix} \hat{i}' \\ \hat{j}' \\ \hat{k}' \end{pmatrix}$$

for each element S of P.

From Sec. II 2.2, it is seen that q_4, q_5, q_6 transform under P like yz, xz, xy respectively. However under P , (yz, xz, xy) transform in turn like (x, y, z). Thus under P , (q_4, q_5, q_6) transform as (x, y, z); hence for a given S

$$\begin{pmatrix} q_4 \\ q_5 \\ q_6 \end{pmatrix} \longrightarrow \tilde{R}_S \begin{pmatrix} q_4 \\ q_5 \\ q_6 \end{pmatrix}$$

From Sec. II 2.2, it is also seen that q_3, q_2 transform like the quantities $\frac{2z^2 - x^2 - y^2}{\sqrt{6}}$, $\frac{x^2 - y^2}{\sqrt{2}}$ respectively.

The column $U^{(22)}(S)$ gives the transformation induced on the column vector $\begin{pmatrix} q_3 \\ q_2 \end{pmatrix}$: under S

$$\begin{pmatrix} q_3 \\ q_2 \end{pmatrix} \longrightarrow U^{(22)}(S) \begin{pmatrix} q_3 \\ q_2 \end{pmatrix}$$

Permutation S	Parity p	Ψ	θ	Ø	R_S	$U^{(22)}(S)$
E	+1	0	0	0	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
(41)	-1	$\frac{-\pi}{2}$	$\frac{\pi}{2}$	$\frac{-\pi}{2}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$
(23)	-1	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$
(42)	-1	π	$\frac{\pi}{2}$	0	$\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}$
(13)	-1	0	$\frac{\pi}{2}$	π	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}$
(43)	-1	$\frac{\pi}{2}$	π	0	$\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
(12)	-1	$\frac{-\pi}{2}$	π	0	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
(41)(23)	+1	$\frac{\pi}{2}$	π	$\frac{-\pi}{2}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
(42)(13)	+1	0	π	0	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
(43)(12)	+1	π	0	0	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Permutation S	Parity p	Ψ	θ	ϕ	R_S	$U^{(22)}(S)$
(234)	+1	0	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$
(243)	+1	$\frac{\pi}{2}$	$\frac{\pi}{2}$	π	$\begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$
(134)	+1	$\frac{-\pi}{2}$	$\frac{\pi}{2}$	0	$\begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$
(143)	+1	π	$\frac{\pi}{2}$	$\frac{-\pi}{2}$	$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$
(124)	+1	0	$\frac{\pi}{2}$	$\frac{-\pi}{2}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$
(142)	+1	$\frac{-\pi}{2}$	$\frac{\pi}{2}$	0	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}$
(132)	+1	π	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$
(1243)	-1	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{-\pi}{2}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$
(1342)	-1	$\frac{-\pi}{2}$	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$
(1234)	-1	π	$\frac{\pi}{2}$	π	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}$
(1432)	-1	0	$\frac{\pi}{2}$	0	$\begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}$
(1423)	-1	$\frac{-\pi}{2}$	0	0	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
(1324)	-1	$\frac{\pi}{2}$	0	0	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

The transformation of angular functions $Y_{J\underline{+}}^{km}(\Gamma)$ under P follows from eq. AI.11. Since the rotation Γ_S corresponding to a permutation S of P is given with respect to the $\hat{i}'$, $\hat{j}'$, $\hat{k}'$ body axes, the permutation S induces on Γ the transformation

$$\Gamma \dashrightarrow \Gamma_S \Gamma \quad ;$$

hence the transformation induced on any $Y_{J\underline{+}}^{km}(\Gamma)$ is:

$$Y_{J\underline{+}}^{km}(\Gamma) \dashrightarrow \sum_{h} Y_{J\underline{+}}^{kh}(\Gamma_S)\, Y_{J\underline{+}}^{km}(\Gamma) \;,$$

and the matrix of the transformation is:

$$Y_{J\underline{+}}^{kh}(\Gamma_S) = (\underline{+}\,1)^{\varphi_S}\, e^{i(k\Psi_S+h\emptyset_S)}\, P_J^{kh}(\theta_S) \quad .$$

Both the transformation $Y_{J\underline{+}}^{kh}(\Gamma_S)$ angular functions and that (such as $\bar{R}$ (S)) on coordinates q_4, q_5, q_6, on vibration functions form right-handed multiplicative groups. That being established makes it necessary in combining functions to consider the transformations induced by the six group generators only.

We take as basis for the standard realizations of the irreducible representations of group P_4 ;

for (211): basis $\begin{pmatrix} Y_{1-}^{1,m} \\ Y_{1-}^{o,m} \\ Y_{1-}^{-1,m} \end{pmatrix}$; representation $U_y^{(211)}(S)$

for (31): basis $\begin{pmatrix} Y_{1+}^{1,m} \\ Y_{1+}^{o,m} \\ Y_{1+}^{-1,m} \end{pmatrix}$; representation

$$U_y^{(31)}(S)=(-1)^{p_S}\, U_y^{(211)}(S)$$

for (22): basis
$$\begin{matrix} v_{2+}^{2,m} = \frac{1}{\sqrt{2}} (Y_{2+}^{2,m} + Y_{2+}^{-2,m}) \\ v_{2+}^{o,m} = Y_{2+}^{o,m} \end{matrix} \quad ;$$

representation $U_y^{(22)}(S)$;

representations (1) and (4) are trivial.

The standard representations $U_y^{(211)}(S)$ and $U_y^{(22)}(S)$ for S in the class (12) are given below. We also include the representation

$U_q^{(211)}(S)$ induced on basis
$$\begin{pmatrix} v_1^1 = -\frac{1}{\sqrt{2}} (q_4 + iq_5) \\ v_1^o = q_6 \\ v_1^{-1} = \frac{1}{\sqrt{2}} (q_4 - iq_5) \end{pmatrix}$$

it is seen that all S of class (12), $U_q^{(211)}(S) = (U_y^{(211)}(S))^*$. It then follows that $U_q^{(211)}(S) = [U_y^{(211)}(S)]^*$ for all S of P, and since the U's are unitary, $[U_2^{(211)}(S)]^T = [U_y^{(211)}(S)]^{-1}$ for all S.

Further the representation $U_q^{(22)}(S)$ induced on $\begin{pmatrix} q_3 \\ q_2 \end{pmatrix}$ also obeys the property $U_q^{(22)}(S) = (U_y^{22}(S))^* = U_y^{22}(S)$. (The last since these matrices have only real elements.) And $[U_q^{(22)}(S)]^T = [U_y^{(22)}(S)]^{-1}$ for all S.

Permutation S	Parity p	Ψ	Θ	$\emptyset$	$U^{(22)}(S)$	$U_q^{(211)}(S)$	$U_y^{(211)}(S)$
41	-1	$\frac{-\pi}{2}$	$\frac{\pi}{2}$	$\frac{-\pi}{2}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 0 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 0 & i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix}$
23	-1	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 0 & -i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 0 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix}$
42	-1	π	$\frac{\pi}{2}$	0	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}$
13	-1	0	$\frac{\pi}{2}$	π	$\frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}$
43	-1	$\frac{\pi}{2}$	π	0	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}$
12	-1	$\frac{-\pi}{2}$	π	0	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 0 \end{pmatrix}$

APPENDIX IV

WAVE FUNCTIONS WHICH BELONG TO THE STANDARD IRREDUCIBLE REPRESENTATION

Since under a permutation S of P, $Y_{J\pm}(\Gamma) \rightarrow Y_{J\pm}(\Gamma_S) Y_{J\pm}(\Gamma)$, the matrix $(Y^{kh}_{J\pm})_\alpha$ which projects $Y_{J\pm}(\Gamma)$ onto the α representation is:

$$(Y^{kh}_{J\pm})_\alpha = \frac{1}{24} \sum_S \chi^{(\alpha)}(S) \, Y^{kh}_{J\pm}(\Gamma_S)$$

$$= \sum_S (\pm 1)^{\theta s} \chi^{(\alpha)}(S) \, e^{i(k\Psi_S + h\emptyset_S)} \, P^{kh}_J(\theta_S)$$

All θ_S are given as 0, $\pi/2$, or π:

$$P^{km}_J(0) = \delta_{km} \, , \qquad P^{km}_J(\pi) = (-1)^{J-k} \, \delta_{k,-m}$$

$P^{km}_J(\frac{\pi}{2})$ are given for $J \leq 4;\ m \geq k \geq 0$.

Other terms $P^{km}_J(\frac{\pi}{2})$ can be found from:

$$P^{k,m}_J = P^{-m,-k}_J = (-1)^{k-m} P^{m,k}_J = (-1)^{k-m} P^{-k,-m}_J = (-1)^{J-k} P^{k,-m}_J$$

$$= (-1)^{J-k} P^{m,-k}_J = (-1)^{J+m} P^{-k,m}_J = (-1)^{J+m} P^{-m,k}_J$$

$$P^{oo}_o(\frac{\pi}{2}) = 1$$

$P^{km}_1(\frac{\pi}{2})$

$$k \;\; \begin{array}{r|cc} 1 & \frac{1}{2} & \\ 0 & -\frac{1}{2} & 0 \\ \hline & 1 & 0 \end{array}$$

$$m$$

$P_2^{km}(\frac{\pi}{2})$

$$\begin{array}{cc|ccc}
 & 2 & \frac{1}{4} & & \\
k & 1 & -\frac{1}{2} & -\frac{1}{2} & \\
 & 0 & \frac{1}{4}\sqrt{6} & 0 & -\frac{1}{2} \\
\hline
 & & 2 & 1 & 0 \\
 & & & m &
\end{array}$$

$P_3^{km}(\frac{\pi}{2})$

$$\begin{array}{cc|cccc}
 & 3 & \frac{1}{8} & & & \\
 & 2 & -\frac{1}{8}\sqrt{16} & -\frac{1}{2} & & \\
k & 1 & \frac{1}{8}\sqrt{15} & \frac{1}{8}\sqrt{10} & -\frac{1}{8} & \\
 & 0 & -\frac{1}{4}\sqrt{5} & 0 & \frac{1}{4}\sqrt{3} & 0 \\
\hline
 & & 3 & 2 & 1 & 0 \\
 & & & m & &
\end{array}$$

$P_4^{km}(\frac{\pi}{2})$

$$\begin{array}{cc|ccccc}
 & 4 & \frac{1}{16} & & & & \\
 & 3 & -\frac{1}{8}\sqrt{2} & -\frac{3}{8} & & & \\
k & 2 & \frac{1}{8}\sqrt{7} & \frac{1}{8}\sqrt{14} & \frac{1}{4} & & \\
 & 1 & \frac{1}{8}\sqrt{14} & -\frac{1}{8}\sqrt{7} & \frac{1}{8}\sqrt{3} & \frac{3}{8} & \\
 & 0 & \frac{1}{16}\sqrt{70} & 0 & -\frac{1}{2}\sqrt{10} & 0 & \frac{3}{8} \\
\hline
 & & 4 & 3 & 2 & 1 & 0 \\
 & & & m & & &
\end{array}$$

Matrices $6(Y^{kh}_{J\pm})_{\alpha}$ for $J \leq 4$ are given in the table which follows: for $J < 4$ only the $(2J + 1)^{th}$ order central portion is applicable.

$(211)^{a}$ or $(31)^{b}$

$\binom{0}{1}$	0	0	0	0	0	0	0	$-(-1)^{J}\binom{0}{1}$
0	$1\mp 2P_{J}^{33}$	0	0	0	$\pm(-1)^{J}2P_{J}^{13}$	0	0	0
0	0	$\binom{1}{0}$	0	0	0	$-(-1)^{J}\binom{1}{0}$	0	0
0	0	0	$1\mp 2P_{J}^{11}$	0	0	0	$\pm(-1)^{J}2P_{J}^{13}$	0
0	0	0	0	$[1-(-1)^{J}]\binom{0}{1}$	0	0	0	0
0	$\pm(-1)^{J}P_{J}^{13}$	0	0	0	$1\mp 2P_{J}^{11}$	0	0	0
0	0	$-(-1)^{J}\binom{1}{0}$	0	0	0	$\binom{1}{0}$	0	0
0	0	0	$\pm(-1)^{J}2P_{J}^{13}$	0	0	0	$1\mp 2P_{J}^{33}$	0
$(-1)^{J}\binom{0}{1}$	0	0	0	0	0	0	0	0

---

[a] Upper/lower signs and bracketed numbers for even/odd parity.

[b] Lower/upper signs and bracketed numbers for even/odd parity.

$(1111)^{a}$ or $(4)^{b}$

$\binom{1}{0}(1+4P_J^{44})$	0	0	0	$(-1)^J\binom{4}{0}P_J^{04}$	0	0	0	$(-1)^J\binom{1}{0}(1+4P_J^{44})$
0	0	0	0	0	0	0	0	0
0	0	$\binom{0}{1}(1-4P_J^{22})$	0	0	0	$(-1)^J\binom{0}{1}(1-4P_J^{22})$	0	0
0	0	0	0	0	0	0	0	0
$\binom{4}{0}P_J^{04}$	0	0	0	$\binom{1}{0}([1+(-1)^J]+4P_J^{00})$	0	0	0	$(-1)^J\binom{4}{0}P_J^{04}$
0	0	0	0	0	0	0	0	0
0	0	$(-1)^J\binom{0}{1}(1-4P_J^{22})$	0	0	0	$\binom{0}{1}(1-4P_J^{22})$	0	0
0	0	0	0	0	0	0	0	0
$(-1)^J\binom{1}{0}(1+4P_J^{44})$	0	0	0	$\binom{4}{0}P_J^{04}$	0	0	0	$\binom{1}{0}(1+4P_J^{44})$

[a] Upper/lower signs and bracketed numbers for even/odd parity.

[b] Lower/upper signs and bracketed numbers for even/odd parity.

(22)

$$\begin{matrix}
1-2P_J^{44} & 0 & 0 & 0 & -(-1)^J 2P_J^{o4} & 0 & 0 & 0 & (-1)^J(1-2P_J^{44}) \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1+2P_J^{22} & 0 & 0 & 0 & (-1)^J(1+2P_J^{22}) & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-2P_J^{o4} & 0 & 0 & 0 & [1+(-1)^J]-2P_J^{oo} & 0 & 0 & 0 & -(-1)^J P_J^{o4} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & (-1)^J(1+2P_J^{22}) & 0 & 0 & 0 & 1+2P_J^{22} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(-1)^J(1-2P_J^{44}) & 0 & 0 & 0 & -2P_J^{o4} & 0 & 0 & 0 & 1-2P_J^{44}
\end{matrix}$$

Normalized wave functions which transform according to the standard representations $U^{(\alpha)}(S)$ or $[U^{(\alpha)}(S)]^*$ are:

$U^{(211)}(S)$:

$$Y_{1-}^{1m}, \quad Y_{1-}^{om}, \quad Y_{1-}^{-1m}$$

$$-Y_{2+}^{-1m}, \quad -\frac{1}{\sqrt{2}}(Y_{2+}^{2m} - Y_{2+}^{-2m}), \quad Y_{2+}^{1m}$$

$$\frac{1}{\sqrt{8}}(\sqrt{5}\,Y_{3+}^{-1,m} - \sqrt{3}\,Y_{3+}^{3,m}), \quad \frac{1}{\sqrt{2}}(Y_{3+}^{2,m} + Y_{3+}^{-2,m}), \quad \frac{1}{\sqrt{8}}(\sqrt{5}\,Y_{3+}^{1,m} - \sqrt{3}\,Y_{3+}^{-3,m})$$

$$\frac{1}{\sqrt{8}}(\sqrt{3}\,Y_{3-}^{1,m} + \sqrt{5}\,Y_{3-}^{-3,m}), \quad -Y_{3-}^{o,m}, \quad \frac{1}{\sqrt{8}}(\sqrt{3}\,Y_{3-}^{-1,m} + \sqrt{5}\,Y_{3-}^{3,m})$$

$$\frac{1}{\sqrt{8}}(\sqrt{7}\,Y_{4+}^{3,m} - Y_{4+}^{-1,m}), \quad \frac{1}{\sqrt{2}}(Y_{4+}^{2,m} - Y_{4+}^{-2,m}), \quad -\frac{1}{\sqrt{8}}(\sqrt{7}\,Y_{4+}^{-3,m} - Y_{4+}^{1,m})$$

$$\frac{1}{\sqrt{8}}(Y_{4-}^{-3,m} + \sqrt{7}\,Y_{4-}^{1,m}), \quad -\frac{1}{\sqrt{2}}(Y_{4-}^{4,m} - Y_{4-}^{-4,m}), \quad \frac{1}{\sqrt{8}}(Y_{4-}^{3,m} + \sqrt{7}\,Y_{4-}^{-1,m})$$

and with the definitions:

$$v_1^1 = -\frac{1}{\sqrt{2}}(q_4 + iq_5) \qquad \frac{1}{\sqrt{2}}(v_2^2 + v_2^{-2}) = \frac{1}{2}\sqrt{3}\,(q_4^2 - q_5^2)$$

$$v_1^o = q_6 \qquad \frac{1}{\sqrt{2}}(v_2^2 - v_2^{-2}) = i\sqrt{3}\,q_4 q_5$$

$$v_1^{-1} = \frac{1}{\sqrt{2}}(q_4 + iq_5) \qquad v_2^1 = -\sqrt{\frac{3}{2}}\,q_6(q_4 + iq_5)$$

$$v_2^o = \frac{1}{2}(2q_1^2 - q_5^2 - q_4^2)$$

$$v_2^{-1} = \sqrt{\frac{3}{2}}\,q_6(q_4 - iq_5)$$

$[U^{(211)}(S)]^*$:

$$v_1^1 \;,\quad v_1^0 \;,\quad v_1^{-1}$$

$$-v_2^{-1} \;,\; -\frac{1}{\sqrt{2}}\,(v_2^2 - v_2^{-2}), \quad v_2^1$$

$$\frac{1}{2}\,(v_1^1\, q_3 + \sqrt{3}\, v_1^{-1}\, q_2), \quad -v_1^0\, q_3 \;,\; \frac{1}{2}\,(v_1^{-1}\, q_3 + \sqrt{3}\, v_1^1\, q_2)$$

$U^{(31)}(S)$:

Change parity of all functions listed under $U^{(211)}(S)$.

$[U^{(31)}(S)]^*$:

$$\frac{1}{2}\,(v_1^1\, q_2 - \sqrt{3}\, v_1^{-1}\, q_3) \;,\; -v_1^0\, q_2 \;,\; \frac{1}{2}\,(v_1^{-1}\, q_2 - \sqrt{3}\, v_1^1\, q_3)$$

$U^{(22)}(S)$:

$$Y_{2+}^{0,m} \;,\; \frac{1}{\sqrt{2}}\,(Y_{2+}^{2,m} + Y_{2+}^{-2,m})$$

$$\frac{1}{\sqrt{2}}\,(Y_{2-}^{2,m} + Y_{2-}^{-2,m}) \;,\quad -Y_{2-}^{0,m}$$

$$\frac{1}{\sqrt{24}}\,(\sqrt{7}\, Y_{4+}^{4,m} - \sqrt{10}\, Y_{4+}^{0,m} + \sqrt{7}\, Y_{4+}^{-4,m}) \;,\; \frac{1}{\sqrt{2}}\,(Y_{4+}^{2,m} + Y_{4+}^{-2,m})$$

$$\frac{1}{\sqrt{2}}\,(Y_{4-}^{2,m} + Y_{4-}^{-2,m}) \;,\quad -\frac{1}{\sqrt{24}}\,(\sqrt{7}\, Y_{4+}^{0,m} - \sqrt{10}\, Y_{4}^{0,m} + \sqrt{7}\, Y_{4+}^{-4,m})$$

$$q_3 \;,\quad q_2$$

$$v_2^0 \;,\quad \frac{1}{\sqrt{2}}\,(v_2^2 + v_2^{-2})$$

$U^{(1111)}(S)$:

$$Y^{oo}_{o+}$$

$$\frac{1}{\sqrt{2}} (Y^{2,m}_{3-} - Y^{-2,m}_{3-})$$

$$\frac{1}{\sqrt{24}} (\sqrt{5}\ Y^{4,m}_{4+} + \sqrt{14}\ Y^{o,m}_{4+} + \sqrt{5}\ Y^{-4,m}_{4+})$$

$U^{(4)}(S)$:

Opposite parity from $U^{(1111)}(S)$.

APPENDIX V

TOTAL WAVE FUNCTIONS FOR $n_2 + n_3 \leq 1, \quad J \leq 4$; $n_2 + n_3 = 2, \quad n_2 \leq 1, \quad J \leq 2.$

The ground state wave function

$$\Psi_o = \exp - \frac{1}{2} \sum_{i=1}^{6} q_i^2$$

is understood as a factor of all wave functions. The factor $H_{n_1}(q_1)$ is not given. Normalization is incomplete. A normalizing factor C_{n_1, n_2, n_3} is to be applied to all wave functions.

$(n_1, n_2, n_3; J\pm) = (0,0,0,0+)$

$$\Psi = 1.$$

(0,0,0,3-)

$$\Psi^m = \frac{1}{\sqrt{2}} (Y_{3-}^{2,m} - Y_{3-}^{-2,m})$$

(0,0,0,4+)

$$\Psi^m = \frac{1}{\sqrt{24}} (\sqrt{5}\ Y_{4+}^{4,m} + \sqrt{14}\ Y_{4+}^{o,m} + \sqrt{5}\ Y_{4+}^{-4,m})$$

(0,1,0,2+)

$$\Psi^m = \frac{1}{2} (\sqrt{2}\ q_3\ Y_{2+}^{o,m} + q_2[Y_{2+}^{2,m} + Y_{2+}^{-2,m}])$$

(0,1,0,2-)

$$\Psi^m = \frac{1}{\sqrt{2}} (\sqrt{2}\ q_2\ Y_{2-}^{o,m} - q_3[Y_{2-}^{2,m} + Y_{2-}^{-2,m}])$$

(0,1,0,4+)

$$\Psi^m = \frac{1}{4\sqrt{3}} (q_3[\sqrt{7}\ Y_{4+}^{4,m} - \sqrt{10}\ Y_{4+}^{o,m} + \sqrt{7}\ Y_{4}^{-4,m}] + \sqrt{24}\ q_2[Y_{4+}^{2,m} + Y_{4+}^{-2,m}])$$

(0,1,0,4-)

$$\Psi^{m} = \frac{1}{4\sqrt{3}}(q_2[\sqrt{7}\ Y_{4-}^{4,m} - \sqrt{10}\ Y_{4-}^{o,m} + \sqrt{7}\ Y_{4-}^{-4,m}] - \sqrt{24}\ q_3[Y_{4-}^{2,m} + Y_{4-}^{-2,m}])$$

(0,0,1,1-)

$$\Psi^{m} = \frac{1}{\sqrt{3}}(v_1^1\ Y_{1-}^{1,m} + v_1^o\ Y_{1-}^{o,m} + v_1^{-1}\ Y_{1-}^{-1,m})$$

$L = 1, \quad \vec{J} \cdot \vec{L} = 2$

(0,0,1,2+)

$$\Psi^{m} = \frac{1}{\sqrt{6}}(\sqrt{2}\ v_1^1\ Y_{2+}^{-1,m} + v_1^o\ [Y_{2+}^{2,m} - Y_{2+}^{-2,m}] - \sqrt{2}\ v_1^{-1}\ Y_{2+}^{1,m})$$

$L = 1 , \quad \vec{J} \cdot \vec{L} = -2$

(0,0,1,3+)

$$\Psi^{m} = \frac{1}{\sqrt{24}}(v_1^1\ [\sqrt{5}\ Y_{3+}^{-3,m} - \sqrt{3}\ Y_{3+}^{3,m}] + \sqrt{12}\ v_1^o\ [Y_{3+}^{2,m} + Y_{3+}^{-2,m}]$$
$$+ v_1^{-1}[\sqrt{5}\ Y_{3+}^{1,m} - \sqrt{3}\ Y_{3+}^{-3,m}])$$

$L = 1 , \quad \vec{J} \cdot \vec{L} = 1$

(0,0,1,3-)

$$\Psi^{m} = \frac{1}{\sqrt{24}}(v_1^1[\sqrt{5}\ Y_{3-}^{-3,m} + \sqrt{3}\ Y_{3-}^{1,m}] - \sqrt{8}\ v_1^o\ Y_{3-}^{o,m}$$
$$+ v_1^{-1}[\sqrt{5}\ Y_{3-}^{3,m} + \sqrt{3}\ Y_{3-}^{-1,m}])$$

$L = 1 , \quad \vec{J} \cdot \vec{L} = -3$

(0,0,1,4+)

$$\Psi^m = \frac{1}{\sqrt{24}} (v_1^1[\sqrt{7}\, Y_{4+}^{3,m} - Y_{4+}^{-1,m}] + 2v_1^o[Y_{4+}^{2,m} - Y_{4+}^{-2,m}]$$

$$- v_1^{-1}[\sqrt{7}\, Y_{4+}^{-3,m} - Y_{4+}^{1,m}])$$

$L = 1$, $\vec{J} \cdot \vec{L} = 5$

(0,0,1,4-)

$$\Psi^m = \frac{1}{\sqrt{24}} (v_1^1[Y_{4-}^{-3,m} + \sqrt{7}\, Y_{4-}^{1,m}] - 2v_1^o[Y_{4-}^{4,m} - Y_{4-}^{-4,m}]$$

$$- v_1^{-1}[Y_{4-}^{3,m} + \sqrt{7}\, Y_{4-}^{-1,m}])$$

$L = 1$, $\vec{J} \cdot \vec{L} = 1$

(0,1,1,1-)

$$\Psi^m = \frac{1}{\sqrt{12}} (\sqrt{2}\, q_3\, [v_1^1\, Y_{1-}^{1,m} - 2v_1^o\, Y_{1-}^{o,m} + v_1^{-1}\, Y_1^{-1,m}]$$

$$+ \sqrt{6}\, q_2[v_1^1\, Y_{1-}^{-1,m} + v_1^{-1}\, Y_{1-}^{1,m}])$$

$L = 1$, $\vec{J} \cdot \vec{L} = -1$

(0,1,1,1+)

replace q_3 by q_2, q_2 by $-q_3$ in above, change parity

$L = 1$, $\vec{J} \cdot \vec{L} = -1$

(0,1,1,2+)

$$\Psi^m = \frac{1}{\sqrt{12}} (\sqrt{2}\, q_3 \left\{-v_1^1\, Y_{2+}^{-1,m} + \sqrt{2}\, v_1^o[Y_{2+}^{2,m} - Y_{2+}^{-2,m}] + v_1^{-1}\, Y_{2+}^{1,m}\right\}$$

$$+ \sqrt{6}\, q_2 \left\{v_1^1\, Y_{2+}^{1,m} - v_1^{-1}\, Y_{2+}^{-1,m}\right\})$$

$L = 1$, $\vec{J} \cdot \vec{L} = 1.$

(0,1,1,2-)

replace q_3 by q_2, q_2 by $-q_3$ in the above, change parity; $L = 1$, $\vec{J} \cdot \vec{L} = 1$.

(0,0,2,0+)

$$L = 0 \ , \quad \Psi^m = \frac{1}{\sqrt{3}} (q_4^2 + q_5^2 + q_6^2 - \tfrac{3}{2})$$

(0,0,2,1-)

$$\Psi^m_S = \frac{1}{\sqrt{6}} (\sqrt{2}\, v_2^{-1}\, Y_{1-}^{1,m} + [v_2^2 - v_2^{-2}]\, Y_{1-}^{o,m} - \sqrt{2}\, v_2^1\, Y_{1-}^{-1,m})$$

$$L = 2 \ , \quad \vec{J} \cdot \vec{L} = -2.$$

(0,0,2,2+)

$L = 2$.

Both the vibrational and the rotational wave functions have a (22) representation and a (211) representation.

From the (22) functions, we form

$$\Psi^m = \frac{1}{2\sqrt{2}} (2v_2^o\, Y_{2+}^{o,m} + [v_2^2 + v_2^{-2}][Y_{2+}^{2,m} + Y_{2+}^{-2,m}]) \ .$$

From the (211) functions, we form

$$\Psi^m_A = \frac{1}{2\sqrt{3}} (v_2^1\, Y_{2+}^{1,m} + [v_2^2 - v_2^{-2}][Y_{2+}^{2,m} - Y_{2+}^{-2,m}] + v_2^{-1}\, Y_{2+}^{-1,m}) \ .$$

Neither is an eigenvalue of $\vec{J} \cdot \vec{L}$:

$$(\vec{J} \cdot \vec{L})\, \Psi^m_S = 2\sqrt{6}\, \Psi^m_A \quad , \qquad (\vec{J} \cdot \vec{L})\, \Psi^m_A = 2\sqrt{6}\, \Psi^m_S + 2\Psi^m_A$$

States

$$\frac{1}{\sqrt{5}} (\sqrt{2}\, \Psi^m_S + \sqrt{3}\, \Psi^m_A) \quad \text{and} \quad \frac{1}{\sqrt{11}} (\sqrt{3}\, \Psi^m_A - 2\sqrt{2}\, \Psi^m_S)$$

are eigenfunctions with $\vec{J} \cdot \vec{L} = 6$ and -4($I = 0^+, 4^+$) respectively.

(0,0,2,2-)

J = 2- functions have no (211) representation, so there is only one state, derived from (22) functions

$$\Psi^{m} = \frac{1}{2}\ (v_{2}^{o}[Y_{2-}^{2,m} + Y_{2-}^{-2,m}] - [v_{2}^{2} + v_{2}^{-2}]\ Y_{2-}^{o,m})$$

$$L = 2\ ,\quad \vec{J}\cdot\vec{L} = 0\quad (I = 3^{-})\ .$$

REFERENCES

[1] G. Herzberg, Molecular Spectra and Molecular Structure, Vol. II, D. Van Nostrand (1945).

[2] E.B. Wilson and J.B. Howard, J. Chem. Phys. 4, 260 (1936).

[3] W.H. Shaffer, J. Chem. Phys. 9, 607 (1941).

[4] B.T. Darling and D.M. Dennison, P.R. 57, 128 (1940).

[5] T. Takehashi, J. Phys. Soc. Jap. 7, 307 (1952).

[6] D.M. Dennison, Phys. Rev. 96, 378 (1954).

[7] F. Ajzenberg, and T. Lauritsen, Rev. Mod. Phys. 24, 321 (1952).

[8] A. Schardt, W.A. Fowler, and C.C. Lauritsen, Phys. Rev. 86, 527 (1952).

[9] A. Kraus, Phys. Rev. 44, 975 (1954).

[10] J.W. Bittner and R.D. Moffat, Phys. Rev. 96, 374 (1954).

[11] F. Ajzenberg, and T. Lauritsen, Appendix B, Quarterly Progress Report 4, Dept. of Phys. Boston University (Sept. 30, 1954).

[12] D.H. Wilkinson and G.A. Jones, Phil. Mag. 44, 542 (1953).

[13] R.P. Feynman, Phys. Rev. 76, 749 (1949); R.P. Feynman, Quantum Electrodynamics, C.I.T. (1953).

[14] S. Devons, Proc. of Phys. Soc. A 67, 134 (1954).

[15] S. Devons, (Private communication to T. Lauritsen, Oct. 19, 1954).

[16] J. Thirion, and V.L. Telegdi, Phys. Rev. 93, 950 (1954).

[17] S. Geschwind, R. Gunther-Mohr, and C.H. Townes, Phys. Rev. 83, 209 (1951).

[18] F. Alder and F.C. Yu, Phys. Rev. 81, 1067 (1951).