A STUDY OF THE SYMMETRY OF THE RELATIVISTIC EQUIVALENT OSCILLATOR AND ITS APPLICATIONS

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A STUDY OF THE SYMMETRY OF THE RELATIVISTIC EQUIVALENT OSCILLATOR AND ITS APPLICATIONS

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PREFACE

The mathematical symmetries of the relativistic equivalent harmonic oscillator are studied. It is shown that the relativistic equivalent oscillator Hamiltonian possesses an SO(4) x SU(2) invariance group and an SO(4,1) x SU(2) dynamical symmetry group. A nuclear model based upon this relativistic equivalent oscillator is used to calculate the Coulomb energies of nuclei. The relativistic corrections to the results of the non-relativistic harmonic oscillator shell model are shown to be of the order of one per cent.

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CHAPTER I

INTRODUCTION

The first part of this work is a study of continuous groups and their relation to the mathematical symmetries of the relativistic equivalent oscillator proposed by Swamy (1). The second part is an application of the relativistic equivalent oscillator in an attempt to see what light the Coulomb energies of nuclei throw on the existence of relativistic motion of nucleons in a nucleus.

The motivation for studying the group structure of the relativistic equivalent oscillator is in keeping with the interest of physicists in recent years in the symmetries and dynamical groups of simple quantum mechanical Hamiltonians which possess exact solutions (2, 3, 4). Study of these happens to be useful in the context of certain symmetries occurring in elementary particle physics. Several papers have appeared on the invariance and non-invariance groups of the non-relativistic hydrogen atom, the approximately relativistic Symmetric Coulomb Hamiltonian, the exact Dirac Coulomb problem, and the non-relativistic harmonic oscillator (5, 6, 7, 8). Of particular interest is the group SO(4,1). It has been shown that the $\nu_{0,\sigma}$ and $\nu_{\frac{1}{2},\sigma}$ representations of the continuous class of irreducible representations of this group are realized by the bound states of the non-relativistic hydrogen atom and the exact Dirac Coulomb problem, respectively. In this thesis, it is shown that the $\pi^{+}_{\frac{1}{2},\frac{1}{2}}$ representation of the discrete class can be realized by the solutions of the relativistic equivalent oscillator problem. The

Dirac Hamiltonian for this latter problem possesses exact solutions, and reduces in the non-relativistic limit to an isotropic harmonic oscillator with spin-orbit coupling of the Thomas-Frenkel form. It is therefore likely to provide an interesting alternative to the hydrogen atom for the study of symmetry groups.

A calculation of Coulomb energies using this equivalent oscillator model is carried out with the hope of finding nuclei for which relativistic corrections are not negligible. To enable comparisons to be made, similar calculations are carried out using both the non-relativistic oscillator and the relativistic equivalent oscillator shell models. Models based on these Hamiltonians relate the Coulomb energy to the nuclear radius. The nuclear radius is determined from experiments, to within a certain uncertainty, for example by electron scattering or μ-mesonic atom X-ray experiments. On the other hand, since the mid-1930's the experimental Coulomb energy differences of mirror nuclei have been taken from β-decay data, or from the Q-values of nuclear reactions. These data were then used to estimate the size of the nucleus. Within the last ten years, isobaric analog states have been discovered in heavy nuclei, resulting in an increase in available data on Coulomb energies and nuclear sizes (9, 10). This explains the recent interest in the study of Coulomb energies and gives a motivation for the application of the relativistic equivalent oscillator.

CHAPTER II

CONTINUOUS GROUP THEORY

In this chapter, we discuss continuous groups, and in particular, those aspects of the subject which are relevant to the symmetries of the various quantum mechanical Hamiltonians, and their applications in physics. The concepts of semisimple Lie algebras, root diagrams, weight diagrams, and irreducible representations will be discussed. Since the groups SO(4) and SU(3) are of particular relevance to non-relativistic, single particle quantum mechanics, and also have connections with the relativistic equivalent oscillator, they will be given special attention.

By continuous groups, we mean groups of transformations defined by continuous, differentiable functions

$$x_i' = f_i(x_1, x_2, \ldots, x_n; a_1, \ldots, a_r) \qquad i = 1,2,3,\ldots,n \tag{1}$$

The numbers $a_1, a_2, \ldots, a_r$ are parameters, fixed values of which define a particular group element. If, starting from the set $a_1^o, a_2^o, \ldots, a_r^o$ of parameters defining the identity transformation, we can reach any element of the group by a continuous path in the parametrization space, then the group is said to be connected to the identity. For such groups there exist differential operators X_i, called the infinitesimal generators, by means of which the finite transformations can be built up by repeated application, starting from the identity transformation. The

connection between the infinitesimal generators and finite transformations was first studied by S. Lie (11), who showed that

$$\phi(x_1',x_2',\ldots,x_n') = e^{a_1X_1 + a_2X_2 + \ldots + a_rX_r}\,\phi(x_1,x_2,\ldots,x_n) \qquad (2)$$

as a part of his first fundamental theorem.

An example of this is the two dimensional, proper rotation group with transformations defined by

$$\begin{aligned} x_1' &= x_1 \cos\phi + x_2 \sin\phi \\ x_2' &= -x_1 \sin\phi + x_2 \cos\phi \end{aligned} \qquad (3)$$

From the fact that

$$x_1' = e^{\phi\left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1}\right)} x_1 \qquad (4)$$

we see that one of the generators is

$$X_1 = x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \qquad (5)$$

The generators form a mathematical algebra (12), called a Lie algebra. To define a Lie algebra, we first give the condition that there exists a basis set of linearly independent elements such that any other element X is a linear combination

$$X = \sum_{i=1}^{r} C_i X_i \qquad (6)$$

Secondly, we require the definition of a rule of combination which satisfies the closure condition

$$[X_k, X_l] = \sum_{m=1}^{r} C_{kl}^{m} X_m \tag{7}$$

where the C_{kl}^{m}, called structure constants, are numbers. Thirdly, the structure constants must satisfy

$$C_{kl}^{m} = - C_{lk}^{m} \tag{8}$$

and

$$\sum_{n=1}^{r} (C_{ln}^{k} C_{mj}^{n} + C_{mn}^{k} C_{jl}^{n} + C_{jn}^{k} C_{lm}^{n}) = 0 \tag{9}$$

The second and third fundamental theorems of Lie show that the infinitesimal generators form a Lie algebra, with the rule of combination taken as the commutator. In particular, Lie was able to prove conversely that if the above relations hold, the X_i are the infinitesimal generators of a continuous group.

In quantum mechanics, Lie algebras are formed by Hermitian operators on Hilbert space. Generally speaking, the operators are not represented by homogeneous functions of first derivatives. They are not, therefore, generators in the sense used by Lie. However, the commutation relations, and the Hermiticity conditions are usually enough to ensure that the operators have matrix elements which are equivalent to those of the Lie generators of a continuous group. Which group and which irreducible representations are realized is determined by the values of certain invariant operators which commute with all the elements of the Lie algebra. For a semisimple Lie algebra, defined in the next paragraph, one of these is the Casimir invariant (13)

$$\underset{\sim}{C} = \sum_{\mu,\nu} g^{\mu\nu} X_\mu X_\nu \tag{10}$$

where

$$g_{\mu\nu} = \sum_{\alpha,\beta} C^{\alpha}_{\mu\beta} C^{\beta}_{\nu\alpha}; \; [\underset{\sim}{C}, X_{\mu}] = 0 \tag{11}$$

When we consider the application of different types of Lie algebras, it turns out that a certain type called a semisimple Lie algebra is of most importance. A semisimple Lie algebra is defined as a Lie algebra which possesses no Abelian invariant subalgebras. An Abelian invariant subalgebra is defined as a subalgebra whose elements commute among themselves and whose commutators with other elements of the Lie algebra are contained in the subalgebra. If the requirement that the elements of the subalgebra commute among themselves is relaxed, the subalgebra is called simply an invariant subalgebra. The very special type of algebra possessing no invariant subalgebras is called a simple Lie algebra.

E. Cartan (14) gave a necessary and sufficient condition for a Lie algebra to be semisimple (Cartan's theorem). The condition is that the matrix formed by the metric tensor of Equation (11) be non-singular.

$$\det (g_{\mu\nu}) \neq 0 \tag{12}$$

He also showed that all semisimple Lie algebras can be written as a direct sum of simple Lie algebras. Hence, the problem of classifying semisimple Lie algebras is reduced to one of classifying simple Lie algebras.

The problem of classifying simple Lie algebras was solved by E. Cartan (12) and B. L. van der Waerden (15). Modern discussions of the problem have been given by G. Racah (16) and C. Fronsdal (17).

The first step is to give the largest number of mutually commuting, linearly independent elements. This number is called the rank of the

algebra, and it is obviously at least one. In standard notation, we then write

$$[H_i, H_j] = 0 \qquad i,j = 1,2,\ldots,l \tag{13}$$

Cartan proved that the remaining basis elements of the simple Lie algebra can be chosen so that they satisfy the relations

$$\begin{aligned} [H_i, E_l] &= r_i(l)\, E_l \\ [E_l, E_{-l}] &= \sum_{i=1}^{l} r_i(l)\, H_i \\ [E_l, E_\beta] &= N_{l\beta}\, E_{l+\beta} \end{aligned} \tag{14}$$

It is customary to label the H's with numbers for subscripts, and the E's with Greek letters. The $r(\alpha)$ are called root vectors and they play an important role in the classification. If we imagine a set of coordinate axes, with the number of axes equal to the rank of the algebra, then an l-dimensional graph showing all of the root vectors is called a root diagram. When the E's are properly normalized, the angle between neighboring root vectors is constant and the diagram is called the symmetric root diagram.

For example, we consider the Lie algebras of the special unitary group in three dimensions, SU(3), and the special orthogonal group in four dimensions, SO(4). Both of these groups have Lie algebras of rank two. However, SO(4) does not have a simple Lie algebra, since its Lie algebra is isomorphic to that of a direct sum of two simple Lie algebras

$$
\begin{aligned}
[J_k, J_l] &= i\varepsilon_{klm} J_m \\
[K_k, K_l] &= i\varepsilon_{klm} K_m \\
[J_k, K_l] &= 0 \qquad k,l,m = 1,2,3.
\end{aligned}
\tag{15}
$$

The defining representation of the group SO(4) is made up of all four by four real matrices with determinant plus one (this is why it is called special) which leave invariant the form

$$x_1^2 + x_2^2 + x_3^2 + x_4^2 .$$

The infinitesimal generators of this group have been given, for example, by Thomas (18) or Bargmann (19). They are

$$
D_{\alpha\beta} = -i\left[x_\alpha \frac{\partial}{\partial x_\beta} - x_\beta \frac{\partial}{\partial x_\alpha}\right] \qquad \alpha,\beta = 1,2,3,4 \tag{16}
$$

and they obey the commutation relations

$$[D_{\alpha\beta}, D_{\gamma\delta}] = i\,\delta_{\alpha\gamma} D_{\beta\delta} + i\,\delta_{\beta\delta} D_{\alpha\gamma} + i\,\delta_{\alpha\beta} D_{\gamma\beta} + i\delta_{\beta\gamma} D_{\delta\alpha} \tag{17}$$

If we define pseudovector operators by the relations

$$
\begin{aligned}
D_{23} &\to L_1 \qquad D_{31} \to L_2 \qquad D_{12} \to L_3 \\
D_{41} &\to M_1 \qquad D_{42} \to M_2 \qquad D_{43} \to M_3
\end{aligned}
\tag{18}
$$

then we get a more transparent form for the commutation relations

$$
\begin{aligned}
[L_i, L_j] &= i\,\varepsilon_{ijk} L_k \\
[M_i, M_j] &= i\,\varepsilon_{ijk} L_k
\end{aligned}
\tag{19}
$$

$$[L_i, M_j] = i\,\varepsilon_{ijk}\,M_k \qquad i,j,k = 1,2,3. \tag{19}$$

ε_{ijk} here is the Levi-Civita symbol, antisymmetric in interchange of any two indices. The local SO(3) x SO(3) structure is brought out by the transformation

$$\vec{J} = \tfrac{1}{2}(\vec{L} + \vec{M}), \quad \vec{K} = \tfrac{1}{2}(\vec{L} - \vec{M}) \tag{20}$$

giving the commutation relations (15).

The symmetric root diagram is shown in Figure 1a, and corresponds to the generators

$$\begin{aligned} H_1 &= J_3 \qquad E_\alpha = \frac{J_1 + i\,J_2}{\sqrt{2}} \qquad E_{-\alpha} = \frac{J_1 - i\,J_2}{\sqrt{2}} \\ H_2 &= K_3 \qquad E_\beta = \frac{K_1 + i\,K_2}{\sqrt{2}} \qquad E_{-\beta} = \frac{K_1 - i\,K_2}{\sqrt{2}} \end{aligned} \tag{21}$$

The group SU(3) is defined as the group formed by all unitary three by three matrices with determinant plus one:

$$U^+U = UU^+ = 1; \ \det U = 1; \ U^+ = \tilde{U}^* \tag{22}$$

These matrices happen to leave invariant the form

$$|x|^2 + |y|^2 + |z|^2$$

The infinitesimal generators which give the symmetric root diagram are

$$H_1 = \frac{1}{2\sqrt{3}}\left(x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y}\right); \quad H_2 = \frac{1}{6}\left(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}\right) - \frac{1}{3}\,z\frac{\partial}{\partial z} \tag{23}$$

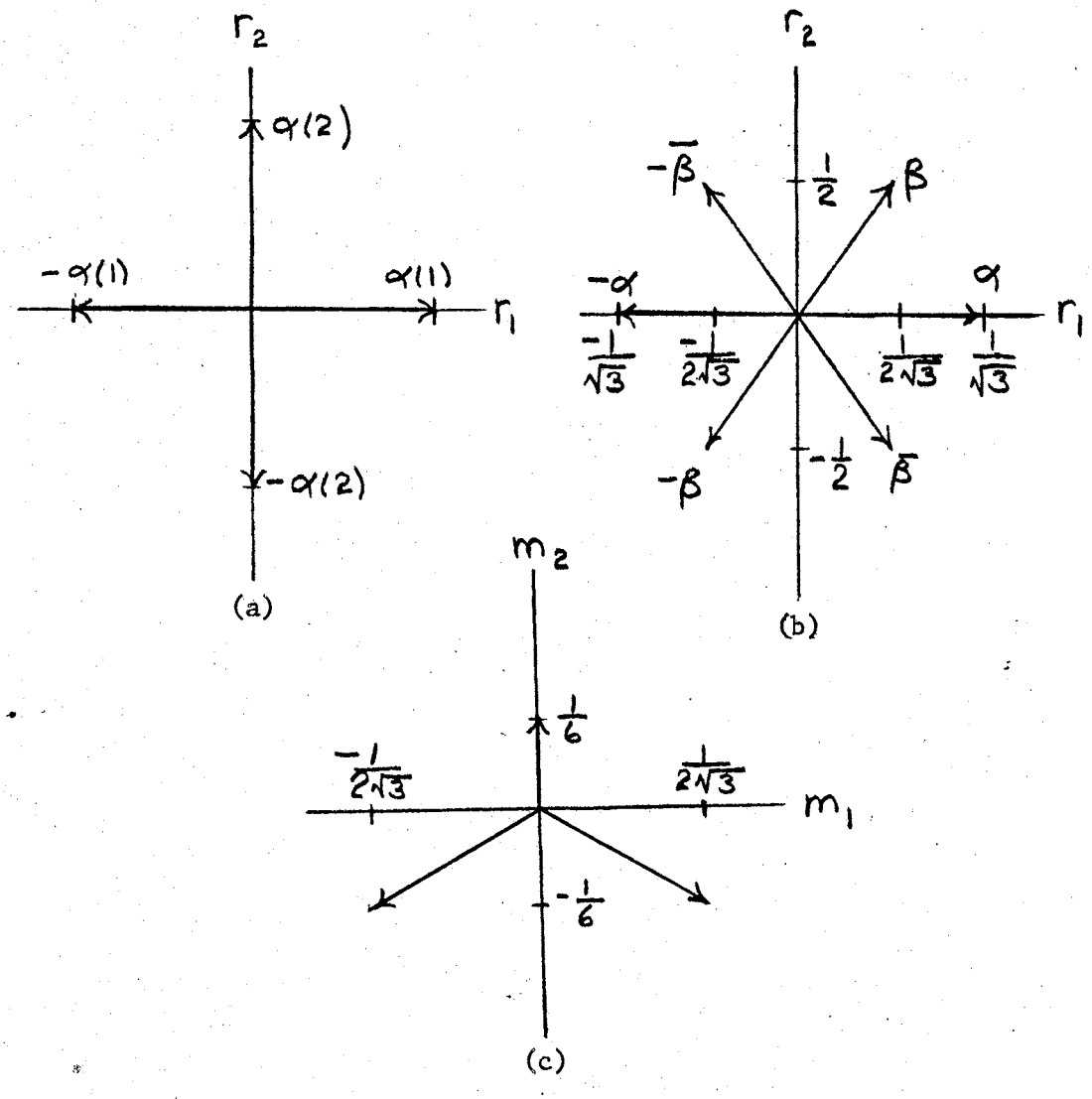

Figure 1. Symmetric Root Diagrams of (a) SO(4) and (b) SU(3). (c) Weight Diagram of the 3 Representation of SU(3)

$$E_{\alpha} = \frac{1}{\sqrt{6}}\ x\frac{\partial}{\partial y};\qquad E_{\beta} = \frac{1}{\sqrt{6}}\ x\frac{\partial}{\partial z};\qquad E_{\bar{\beta}} = \frac{1}{\sqrt{6}}\ z\frac{\partial}{\partial y} \tag{23}$$

$$E_{-\alpha} = \frac{1}{\sqrt{6}}\ y\frac{\partial}{\partial x};\qquad E_{-\beta} = \frac{1}{\sqrt{6}}\ z\frac{\partial}{\partial x};\qquad E_{-\bar{\beta}} = \frac{1}{\sqrt{6}}\ y\frac{\partial}{\partial z}$$

When we say that these operators are the generators, a certain parametrization is assumed. Finite transformations are generated by

$$U = e^{i(\varepsilon_1 H_1 + \varepsilon_2 H_2 + \varepsilon_\alpha E_\alpha + \varepsilon^*_{+\alpha} E_{-\alpha} + \varepsilon_\beta E_\beta + \varepsilon_\beta^* E_{-\beta} + \varepsilon_{\bar{\beta}} E_{\bar{\beta}} + \varepsilon^*_{+\bar{\beta}} E_{-\bar{\beta}})} \tag{24}$$

where ε_1 and ε_2 are real and ε_α, ε_β, $\varepsilon_{\bar{\beta}}$ are complex.

Now that we have this example, we are in a position to explain the $N_{\alpha\beta}$'s of Equation (14). The root diagram of SU(3) is shown in Figure 1b. All the commutation relations are given by this diagram, by reading off the root vectors and a knowledge that

$$N_{\alpha\beta} = \pm\frac{1}{\sqrt{6}} \text{ or } 0 \qquad \alpha \neq -\beta \tag{25}$$

If the vector $\vec{\alpha} + \vec{\beta} = \vec{\gamma}$ is on the root diagram, then $N_{\alpha\beta} \neq 0$. The $\alpha = -\beta$ cases are given by the root vectors as

$$\begin{aligned} [E_\alpha, E_{-\alpha}] &= \frac{1}{\sqrt{3}} H_1 \\ [E_\beta, E_{-\beta}] &= \frac{1}{2\sqrt{3}} H_1 + \frac{1}{2} H_2 \\ [E_{\bar{\beta}}, E_{-\bar{\beta}}] &= \frac{1}{2\sqrt{3}} H_1 - \frac{1}{2} H_2 \end{aligned} \tag{26}$$

We now go to the irreducible representations of semisimple Lie groups, and their pictorial labelings by means of weights and weight diagrams.

Let us recall the case of the SU(2) group. There the irreducible representation is specified uniquely by giving the value of j, which may take on integer or half integer values. The linearly independent basis functions are $2j + 1$ in number, and may be taken to be eigenfunctions of $H_1 = J_z$. If we take $\hbar = 1$, the largest eigenvalue of H_1 is equal to j. Eigenvalues $-j, -j + 1, -j + 2, \ldots, j - 1, j$ also exist. SU(2) has a simple Lie algebra of rank one.

If the rank of the Lie algebra is some number $\ell > 1$, we generalize this by saying that there exists a highest weight vector $(\lambda_1, \lambda_2, \ldots, \lambda_\ell)$ which specifies the irreducible representation uniquely (up to equivalence). Other weight vectors are the labels for basis functions besides the one corresponding to the highest weight vector. The components of the weight vectors are defined by the relations

$$H_i \, \psi(\vec{\lambda}) = \lambda_i \, \psi(\vec{\lambda}) \tag{27}$$

where ψ is a basis function.

For a given irreducible representation, a graph showing the weight vectors is called a weight diagram. Figure 1c, for example, shows the weight diagram for the defining three by three irreducible representation of SU(3), and this representation is sometimes denoted 3.

A more detailed discussion of weights and weight diagrams can be found in the articles by Fronsdal (17), Racah (16), or van der Waerden (15).

Let us now discuss the examples SO(4) and SU(3), that is, their

irreducible representations.

Suppose we have a set of Hermitian operators which satisfy the commutation relations (19) of SO(4). Finding the matrix elements of these operators is equivalent to the problem of finding matrix representations of the Lie algebra of the group SO(4). These matrices then generate representations of the group SO(4) (but not necessarily single valued representations). If we require each basis function to be connected to all the others by the operators of Equation (19), then we are finding "irreducible" representations. The solution of this problem for SO(4) has been discussed by a number of authors, including Pauli (20).

We first find matrix elements of the subalgebra

$$[L_k, L_l] = i \epsilon_{klm} L_m \tag{28}$$

This can be done, as is well known, by appealing to

(1) Commutation relations

(2) Hermiticity conditions

(3) The value of the Casimir invariant:

$$L^2 = L_x^2 + L_y^2 + L_z^2 = L_z^2 + \frac{1}{2}(L_+L_- + L_-L_+) \tag{29}$$

where

$$L_+ = L_x + i L_y; \quad L_- = L_x - i L_y,$$

the well known step up and step down ladder operators in the quantum mechanical theory of angular momentum. The derivation can be found in the book by Merzbacher (21) or the paper by Nelson (22). The result is that, with standard choices of phases, the only non-vanishing matrix

elements are

$$\langle j,\mu|L_z|j,\mu\rangle = \mu$$
$$\langle j,\mu \pm 1|L \pm | j,\mu\rangle = \sqrt{(j \pm \mu)(j \pm \mu + 1)} \tag{30}$$

where $j = 0,\frac{1}{2},1,\ldots$ and $\mu = -j,-j+1,\ldots,j-1,j$, and the SU(2) Casimir invariant is

$$\langle j,\mu|L^2|j,\mu\rangle = j(j+1) \tag{31}$$

In order to find the non-vanishing matrix elements of the operator $\vec{M}$ (defined as a Hermitian operator satisfying Equation (19), we now observe that the Casimir invariant and the second invariant of the SO(4) algebra are:

$$\begin{aligned} C(1) &= \tfrac{1}{2}(\vec{M}\cdot\vec{M} + \vec{L}\cdot\vec{L}) \\ C(2) &= \vec{M}\cdot\vec{L} \end{aligned} \tag{32}$$

One method, used by Condon and Shortley (23), is to now take advantage of the identity

$$(L^2,[L^2,\vec{M}]) = 2(L^2\vec{M} + \vec{M}L^2) - 4\vec{L}(\vec{M}\cdot\vec{L}) \tag{33}$$

or

$$L^4\vec{M} - 2L^2\vec{M}L^2 + \vec{M}L^4 = 2(L^2\vec{M} + \vec{M}L^2) - 4(\vec{M}\cdot\vec{L}) \tag{34}$$

Using the fact that the invariant C(2) must be diagonal within an irreducible representation we then get the result

$$[(j + j' + 1)^2 - 1][(j - j')^2 - 1]\,\langle \alpha j\mu|\vec{M}|\alpha' j'\mu'\rangle = 0 \tag{35}$$

Which implies that the only non-vanishing matrix elements occur for

$$j' = j \pm 1 \quad \text{Or} \quad j' = j \tag{36}$$

With this knowledge, we next use the commutation relation

$$[M_-, J_-] = 0 \tag{37}$$

to get the identity

$$\frac{\langle \alpha\, j\, \mu | M_- | \alpha'; j-1, \mu+1 \rangle}{\sqrt{(j-\mu-1)(j-\mu)}} = \frac{\langle \alpha\, j\, \mu-1 | M_- | \alpha'; j-1, \mu \rangle}{\sqrt{(j-\mu)(j-\mu+1)}} \tag{38}$$

Since each side of this equation is independent of μ, we conclude

$$\langle \alpha\, j\, \mu | M_- | \alpha'\, j+1, \mu+1 \rangle = -\langle \alpha j || \vec{M} || \alpha' j+1 \rangle \sqrt{(j+\mu+1)(j+\mu+2)} \tag{39}$$

where $\langle \alpha j || \vec{M} || \alpha; j+1 \rangle$ is a reduced matrix element, independent of μ.

Similar commutation relations such as

$$[L_+, M_-] = 2\, M_z \tag{40}$$

and the Hermiticity conditions can be used for other matrix elements. In order to finally fix the reduced matrix elements we use the commutation relation

$$[M_+, M_-] = 2\, L_z \tag{41}$$

and the value of C(2). This gives, for example, the equation

$$|\langle j \| \vec{M} \| j-1 \rangle|^2 = \frac{1}{4j^2-1}\left[2C(1) + 1 - \frac{(C(2))^2}{j^2} - j^2 \right] \tag{42}$$

Now

$$|\langle j || \vec{M} || j-1 \rangle|^2 \geq 0 \tag{43}$$

and hence this, together with the fact that the right hand side of the above Equation (42) becomes negative for large j, implies that there must exist a maximum value of j within an irreducible representation. If we therefore choose the phases appropriately, and write the Casimir invariants as

$$C(1) = \frac{1}{2}(j_1^2 - \frac{3}{4}); \quad C(2) = j_o^2 j_1^2 \tag{44}$$

then we get

$$M_\pm|j,\mu\rangle = \pm\sqrt{(j\mp\mu)(j\mp\mu-1)}\,C_j|j-1,\mu\pm1\rangle - \sqrt{(j\mp\mu)(j\pm\mu+1)}\,A_j|j,\mu\pm1\rangle$$
$$\pm\sqrt{(j\pm\mu+1)(j\pm\mu+2)}\,C_{j+1}|j+1,\mu\pm1\rangle$$

$$M_z|j,\mu\rangle = \sqrt{(j+\mu)(j-\mu)}\,C_j|j-1,\mu\rangle - \mu A_j|j,\mu\rangle \tag{45}$$
$$-\sqrt{(j+\mu+1)(j-\mu+1)}\,C_{j+1}|j+1,\mu\rangle$$

where

$$A_j = \frac{-j_o j_1}{j(j+1)} \qquad C_j = \frac{i}{j}\sqrt{\frac{(j^2-j_o^2)(j_1^2-j^2)}{4j^2-1}} \qquad i = \sqrt{-1}$$

Here j_o becomes the lowest value of j within an irreducible representation and j_1 is one plus the highest value. The label α has been dropped since we postulate no higher symmetry than SO(4), hence there can be no extra labels.

The dimensionality of an irreducible representation is now easily seen to be the sum

$$d = \sum_{j=j_o}^{j_1-1}(2j+1) = (j_1-j_o)(j_1+j_o) = j_1^2 - j_o^2 \tag{46}$$

If we define new variables k and l by the equations

$$j_1 = k + \ell + 1 \qquad j_o = |k-\ell| \tag{47}$$

we get

$$d = (2k+1)(2\ell+1) \quad k,\ell = 0,\frac{1}{2},1,\frac{3}{2},\ldots. \tag{48}$$

This result could have been expected from the fact that SO(4) has a Lie algebra which is isomorphic to that of SU(2) x SU(2).

We have thus constructed the Hermitian irreducible representations of the Lie algebra of SO(4). These representations were found in a basis in which L_z and the invariant operators C(1) and C(2) were diagonal. Alternatively, we could have diagonalized the operators H_1 and H_2 which correspond precisely to the decomposition suggested earlier in the discussion of weights. However, we would not then have a basis which is the same as the one needed in Chapter III.

Now consider the SU(3) example. We could follow a procedure similar to that outlined above for SO(4). This has been done, for example, by Nelson (22), who chose a basis in which the isospin operators T^2, T_z and the hypercharge operator U were diagonal. Instead, we choose the following procedure, which has a closer connection with weight vectors and basis functions.

The highest weight of an SU(3) representation is given by (Carruthers (22))

$$(\frac{p+q}{2\sqrt{3}}, \frac{p-q}{6}) \tag{49}$$

where p and q are positive integers or zero. It has been shown by

various authors (Weyl (25), de Swart (26), Fäldt (27) that there exists a simple scheme of tensor basis functions, with p upper and q lower indices, for the irreducible representations of SU(3). We first define a vector by the transformation

$$\bar{x}^i = \sum_{j=1}^{3} \alpha_{ij} x^j \qquad i = 1, 2, 3. \tag{50}$$

where α is any of the three dimensional irreducible representation matrices. The complex conjugate is then denoted by

$$x_i = (x^i)^* \tag{51}$$

It happens that these complex conjugate vectors form a basis for the conjugate representation 3* of SU(3), as do the pseudovectors

$$\xi_i = \frac{1}{2} \epsilon_{ijk} C^{jk} \tag{52}$$

where $$C^{jk} = x^j y^k - x^k y^j$$

This means that

$$\bar{\xi}_j = \alpha^*_{ij} \xi_j = \alpha^{-1}_{ji} \xi_j \tag{53}$$

With this notation in mind, we develop rules for constructing tensor basis functions for irreducible representations of higher dimensionality. The rules are:

(1) The tensor must be totally symmetric in all p upper indices.

(2) The tensor must be totally symmetric in all q lower indices.

(3) The tensor must be traceless ((1) and (2) imply that there must be only one trace, that is, contraction of only one lower and one upper index).

The rigorous proof will not be given here but it is based upon the following arguments. Given a tensor A with p upper and q lower indices, we define new tensors B, C, and D by the relations

$$\begin{aligned} B^{\beta\cdots\delta}_{j\cdots l} &= \delta^{i}_{\alpha} A^{\alpha\beta\cdots\delta}_{ij\cdots l} \\ C^{\gamma\cdots\delta}_{\mu ij\cdots l} &= \tfrac{1}{2} \epsilon_{\mu\alpha\beta} A^{\alpha\beta\gamma\cdots\delta}_{ij\cdots l} \\ D^{m\alpha\beta\cdots\delta}_{k\cdots l} &= \tfrac{1}{2} \epsilon^{mij} A^{\alpha\beta\cdots\delta}_{ijk\cdots l} \end{aligned} \tag{54}$$

The representation formed by the subset of the components of A which are linearly independent is reducible unless B, C, and D are identically zero. Hence, if we mind our p's and q's, we are led to the rules (1), (2), and (3).

These rules lead to formulas for the reduction of direct product representations. For example,

$$x^i y^j z^k = S^{ijk} + F^{ijk} + G^{ijk} + A^{ijk} \tag{55}$$

where

$$\begin{aligned} S^{ijk} &= \tfrac{1}{6}[x^i y^j z^k + x^i y^k z^j + x^j y^i z^k + x^k y^j z^i + x^j y^k z^i + x^k y^i z^j] \\ F^{ijk} &= \tfrac{1}{3}[(x^i z^k - x^k z^i)\, y^j + (y^i z^k - y^k z^i)\, x^j] \\ G^{ijk} &= \tfrac{1}{3}[(x^i y^j - x^j y^i)\, z^k + (y^j z^i - y^i z^j)\, x^k] \\ A^{ijk} &= \tfrac{1}{6}[x^i y^j z^k - x^i y^k z^j - x^j y^i z^k - x^k y^j z^i + x^j y^k z^i + x^k y^i z^j] \end{aligned} \tag{56}$$

is equivalent to the reduction formula

$$3 \otimes 3 \otimes 3 = 10 + 8 + 8 + 1 \tag{57}$$

Here the numbers denote dimensionalities of irreducible representations, and the numbers on the right hand side of the equation are the numbers of linearly independent components of the tensors S, F, G, and A, respectively.

Other results connected with these tensors include the dimensionality formula for irreducible representations of highest weight given by p and q. This is found by first considering a symmetric tensor with only upper indices. The indices can only be 1,2,3. Suppose that m of them are equal to one. Then because the tensor is symmetric, the number of linearly independent components is p - m + 1, which is true since 0,1,2,..., or p - m of the remaining indices may be 2. The total number of linearly independent components is then given by

$$N_1 = \sum_{m=o}^{p} (p - m + 1) = \frac{1}{2}(p + 1)(p + 2) \tag{58}$$

If we now allow the tensor to have q lower indices, and temporarily ignore the restriction that the tensor must be traceless (or actually be a trace in the case of one dimensional representations), the number becomes

$$N_2 = \frac{1}{4}(p + 1)(p + 2)(q + 1)(q + 2) \tag{59}$$

The trace has p-1 upper indices and q-1 lower indices, hence, we have to subtract

$$N_3 = \frac{1}{4}(p)\ (p + 1)\ q\ (q + 1) \tag{60}$$

This finally gives the dimensionality formula

$$d = (1 + p)(1 + q)(1 + \tfrac{1}{2}(p + q)) \tag{61}$$

This result was given by de Swart (26) by this method, but it has been obtained by other authors by other methods. For example, Nelson (22) derived it after constructing irreducible Hermitian representations of the Lie algebra of SU(3).

CHAPTER III

GROUP STRUCTURE OF THE RELATIVISTIC EQUIVALENT OSCILLATOR

This chapter is devoted to the invariance and noninvariance groups of the relativistic equivalent oscillator. We begin by discussing the meaning of these terms, and the related problems that have been solved previously. The work of Fradkin and Kiefer (7) on the one hand, and Malkin and Manko (6, 28) on the other, will be discussed in detail. These authors discussed the relativistic hydrogen atom, hence their work will serve as an introduction to the results presented in the final sections of this chapter, that is, the group structure of the relativistic equivalent oscillator.

It is well known that the existence of degenerate energy levels for various quantum mechanical systems can be connected with the fact that certain operators commute with the Hamiltonian. In addition, the basis functions belonging to any given energy level usually can be shown to realize an irreducible representation of a Lie group, which is called the invariance group of the Hamiltonian. A set of operators then exists which have the commutation relations of the Lie algebra of this group.

When slight perturbation terms are added to the Hamiltonian, the invariance group is usually destroyed. However, as a part of a larger non-invariance group, it is still very relevant to the problem. In

their discussion of the problems of applying group theory to elementary particle physics, Barut (29) and Bohm (3) introduced the idea of a dynamical symmetry group. As used by them, the term applies to a Lie group for which the set of all eigenfunctions of the Hamiltonian provides a basis for one irreducible representation. In addition, the invariance group is required to be a subgroup of the larger group. If the number of energy levels is infinite, it follows that the dynamical symmetry group is non-compact (a compact Lie group is a Lie group whose parameters vary over a finite range). This fact follows from the theorem which states that the unitary irreducible representations of a Lie group cannot be finite dimensional unless the group is compact.

The Lie algebra of the dynamical symmetry group is constructed, of course, by including operators which do not commute with the Hamiltonian. These usually involve non-invariant (i.e., not commuting with the Hamiltonian) generators which take degenerate set of eigenfunctions belonging to a given energy level into these of another level. These thus help mapping of one subspace of the Hilbert space into another subspace. The commutation relations of the Lie algebra may be realized, not identically, but only on functions which are linear combinations of eigenfunctions of the Hamiltonian. That is, the Lie algebra is realized only when the commutators operate in the space for which the solutions form a complete set. This point has been discussed by Malkin and Manko (2).

There does not seem to exist a general, infallible method for finding these invariance and non-invariance groups. Hence, we have to discuss different cases. In non-relativistic quantum mechanics, invariant operators can be found by (A) generalizing classical integrals of the

motion or (B) picking out the operators which enable a separation of variables to be made. The first method is based upon the correspondence between Poisson brackets in classical mechanics and commutators in quantum mechanics.

$$\{F,G\} \rightarrow \frac{1}{i\hbar} [\hat{F},\hat{G}] \tag{1}$$

The second method corresponds, for example, to the existence of the invariant operators

$$A_{ij} = \frac{1}{2m} p_i p_j + \frac{1}{2} m_o \omega^2 x_i x_j \quad i,j = 1,2,3 \tag{2}$$

which exist for the non-relativistic isotropic harmonic oscillator due to separability in Cartesian coordinates.

Neither of these methods works for the relativistic equivalent oscillator. This is connected with the fact that the Dirac matrices do not have a classical analog.

Malkin and Manko (6) discussed the discrete spectrum ($E < m$) for the exact Dirac Coulomb problem and the symmetric Coulomb problem of Biedenharn and Swamy (5). In a second paper, they discussed the continuous spectrum ($E > m$) (28). They showed that $O(4,2) \times SU(2)$ is a dynamical symmetry group for the discrete spectrum of both problems. For the continuous spectrum, $SL(2,c) \times SU(2)$ was shown to be an invariance group of the Biedenharn model.

As an alternative, Kiefer and Fradkin (7) showed that $O(4,1)$ is a dynamical symmetry group for the bound state solutions of both problems.

The difference between the two problems lies in the fact that the $SO(4)$ subgroup is an invariance group only for the symmetric Coulomb problem. For both problems, the $SU(2)$ generators

$$\vec{J} = \vec{r} \times \vec{p} + \tfrac{1}{2}\vec{\sigma} \tag{3}$$

commute with the Hamiltonian. For the exact Dirac problem, however, we have in addition only the Lippman-Johnson operator

$$S = -\left[i\kappa\rho_1 (H - \rho_3) + \gamma(\vec{\sigma}\cdot\hat{r}) \right] \frac{1}{\sqrt{\kappa^2 H^2 - \gamma^2}} \tag{4}$$

where

$$\kappa = \rho_3(\vec{\sigma}\vec{L} + 1) \tag{5}$$

When $|\kappa| \neq N$, this operator causes a doubling of the degeneracy. For the Biedenharn-Swamy problem there exists a "helicity" operator analogous to the above, but there exist in addition other invariant operators (5).

The Malkin and Manko treatment of the discrete spectrum of these two problems was based upon a generalization of their earlier treatment of the nonrelativistic Coulomb problem. This, in turn, was based upon the pioneer work of Fock (30) and Bargman (19). In this approach, we write the Schrodinger equation in momentum space, and then use the Fock variables (defined in a subspace of the Hilbert Space corresponding to $H \to E$)

$$\vec{\zeta} = \frac{2p_0}{p_0^2 + p^2}\vec{p}\,, \quad \zeta_4 = \frac{p_0^2 - p^2}{p_0^2 + p^2}\,, \quad p_0 = \sqrt{-2E} \tag{6}$$

The solutions of the Schordinger equation then correspond to harmonic polynomials of the four variables ζ_i, that is, they are also solutions of the four dimensional Laplace equation

$$\Delta_4 \Phi = \frac{\partial^2\Phi}{\partial\zeta_1^2} + \frac{\partial^2\Phi}{\partial\zeta_2^2} + \frac{\partial^2\Phi}{\partial\zeta_3^2} + \frac{\partial^2\Phi}{\partial\zeta_4^2} = 0 \tag{7}$$

Malkin and Manko showed that fifteen operators corresponding to generators of the O(4,2) group existed, and these operators commuted with the above four dimensional Laplacian when operating on solutions. The next step was the addition of the Pauli spin matrices, which gives the dynamical symmetry group O(4,2) x SU(2), because the SU(2) generators (Pauli Spin Operators) commute with the generators of the O(4,2) group.

The generalization of the above to relativistic problems consists of first writing the iterated symmetric Hamiltonian in the form

$$Q\Phi_E = O_+ O_- \Phi_E = \left(\Delta + \frac{2\alpha Z E}{r} + E^2 - m^2 \right) \Phi_E = 0 \qquad (8)$$

When this equation is transformed to momentum space, the substitution

$$p_o = \sqrt{m^2 - E^2} \qquad (9)$$

leads to an equation of the same form as the Schrodinger equation in momentum space. Since all the Dirac matrices commute with this new equation, the new equation has dynamical symmetry O(4,2) x SU(2,2). The SU(2,2) is generated by the Dirac matrices as against the Pauli matrices which generate SU(2). This similarity of equations enabled Malkin and Manko to conclude that the solutions for the discrete spectrum of both the Biedenharn model and the exact Dirac equation must provide a basis for irreducible representations of the O(4,2) x SU(2) dynamical symmetry group.

The success of the method of Fradkin and Kiefer was based upon a familiarity with the irreducible representations of O(4,1), especially in the basis given by Strom (31). We first observe that the quantum numbers take on the values

$$N = 1, 2, 3, \ldots$$

$$K = -N, N+1, \ldots, -1, +1, \ldots, N-1 \qquad (10)$$

$$\mu = -|K|+\tfrac{1}{2}, \ldots, |K|-\tfrac{1}{2}$$

We next note that these quantum numbers have a one to one correspondence with the numbers used by Strom to label the irreducible representation $\nu_{\frac{1}{2},\sigma}$.

$$\begin{aligned} p &= \frac{S(K)}{2} = +\tfrac{1}{2}, -\tfrac{1}{2} \\ n &= N - \frac{S(K)}{2} = \tfrac{3}{2}, \tfrac{5}{2}, \cdots \\ j &= |K|-\tfrac{1}{2} = \tfrac{1}{2}, \tfrac{3}{2}, \ldots, N-\frac{S(K)}{2}-1 \\ m &= \mu = -|K|+\tfrac{1}{2}, \ldots, |K|-\tfrac{1}{2}. \end{aligned} \qquad (11)$$

By looking at the matrix elements of the Lie algebra we verify that these values are actually assumed by the Strom parameters. Hence, based on this correspondence between the Hilbert space of solutions and the Hilbert space for the irreducible representations, we conclude that the O(4,1) group is a dynamical symmetry group.

The next step followed by Fradkin and Kiefer was to proceed with an explicit construction of the generators. These generators are to satisfy the commutation relations of the SO(4,1) Lie algebra

$$[J_k, J_\ell] = i\epsilon_{k\ell m} J_m \; ; \; [J_k, T] = 0 \; ; \; [N_k, M_\ell] = i\delta_{k\ell} T \qquad (12)$$

$$[J_k, N_\ell] = i\epsilon_{k\ell m} N_m \; ; \; [J_k, M_\ell] = i\epsilon_{k\ell m} M_m \; ; \; [N_k, T] = i M_k$$

$$[M_k, M_\ell] = i\epsilon_{k\ell m} J_m \; ; \; [N_k, N_\ell] = -i\epsilon_{k\ell m} J_m \; ; \; [M_k, T] = i N_k \qquad (13)$$

Since the explicit representation of these operators is complicated and not too relevant for our purpose, we will not go into this here.

We now take up the discussion of the relativistic equivalent oscillator. In the notation of Swamy (1) and with the help of the oscillator "helicity" operator (32) the Hamiltonian can be made to simulate free particle Hamiltonian

$$\underset{\sim}{H} = \rho_1 \vec{\sigma}\cdot\vec{b} + \rho_3 m_o \tag{14}$$

where

$$\vec{\sigma}\cdot\vec{b} = \vec{\sigma}\cdot\vec{p} + i\lambda^2 \vec{\sigma}\cdot\vec{r}\,\frac{\vec{\sigma}\cdot\vec{L}+1}{|\vec{\sigma}\cdot\vec{L}+1|} \tag{15}$$

The normalized solutions are

$$\Phi_{\nu K\mu} = \begin{bmatrix} \sqrt{\frac{E+m_o}{2E}}\,|\nu K\mu\rangle \\ \\ S(K)\sqrt{\frac{E-m_o}{2E}}\,|\nu -K\mu\rangle \end{bmatrix} \tag{16}$$

where $|\nu K\mu\rangle \rightarrow F_{\nu l}\,\chi^{\mu}_{K}$; $|\nu -K\mu\rangle \rightarrow F_{\nu l(-K)}\,\chi^{\mu}_{-K}$

The $F_{\nu l}$ are the non-relativistic isotropic harmonic oscillator radial wave functions

$$F_{\nu l}(r) = \sqrt{\frac{2\lambda^{2l+3}\,\Gamma(\nu+l+3/2)}{\nu!\,[\Gamma(l+3/2)]^2}}\; r^l\, e^{-\frac{(\lambda r)^2}{2}}\; {}_1F_1(-\nu,\, l+\tfrac{3}{2};\, (\lambda r)^2) \tag{17}$$

normalized $\int_0^\infty F_{\nu l}^2\, r^2\, dr = 1$ and

we have used the confluent hypergeometric function

$${}_1F_1(a,b;x) = 1 + \frac{a}{b}x + \frac{a(a+1)}{b(b+1)}\frac{x^2}{2!} + \cdots \tag{18}$$

The χ^{μ}_{K} spin-angle functions (33) are given by the Clebsch-Gordan sum

$$\chi^{\mu}_{K} = \sum_{\tau=-\frac{1}{2},\frac{1}{2}} C^{\ell(K)\,\frac{1}{2}\,j}_{\mu-\tau,\,\tau,\,\mu}\; Y^{\mu-\tau}_{\ell(K)}(\theta,\phi)\; \chi^{\tau}_{\frac{1}{2}} \tag{19}$$

where $\chi^{1/2}_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi^{-\frac{1}{2}}_{1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

We note in passing that the momentum space transformations of the problem happen to provide no further insight into the group structure. In fact, if we transform the wave functions to momentum space, we get

$$\psi_{\nu K\mu}(\vec{p}) = (-1)^{\nu} i^{-\ell} \begin{bmatrix} \sqrt{\frac{E+m_0}{2E}}\,|\nu K\mu\rangle \\ -i\sqrt{\frac{E-m_0}{2E}}\,|\nu -K\mu\rangle \end{bmatrix} \tag{20}$$

Except for different phases for the small and large components, the solutions have the same form.

The energy is given by

$$E = \sqrt{m_0^2 + 4\lambda^2(\nu+|K|+\tfrac{1}{2})} \qquad \begin{matrix} \nu = 0,1,2,\ldots \\ K = \pm 1, \pm 2, \pm 3, \ldots \end{matrix} \tag{21}$$

Since $2j+1 = 2|\kappa|$, the degeneracy of an energy level is given by

$$\begin{aligned} d &= \sum_{K=-1}^{-n-1} 2|K| + \sum_{K=1}^{n+1} 2|K| = 2\sum_{K=1}^{n+1} 2|K| \\ &= 4\,\frac{(n+1)(n+2)}{2} = 2(n+1)(n+2) \end{aligned} \tag{22}$$

This formula suggests the invariance group of the Hamiltonian. We first

find the dimensionality formulas for the irreducible representations of the groups Sp(2n), SU(n), SO(2n), SO(2n+1), G_2, and the other exceptional semisimple Lie groups. These formulas have been given by Weyl (34), Neéman (35), Fronsdal et. al. (36) and other authors. From looking at these formulas, we eliminate all groups except SU(3) and SO(4). The degeneracy of the energy levels happens to be four times the dimensionality of the (p,q) = (n,0) irreducible representations of SU(3) (Equation (61), Chapter II), and twice the degeneracy of a certain series of irreducible representations of SO(4) (Equation (48), Chapter II). Hence, we suspect that SU(3) x SU(2) x SU(2) or SO(4) x SU(2) is the invariance group of this Hamiltonian.

We now show that SO(4) happens to be applicable. To do this, we look for invariant operators which correspond to the generators.

The angular momentum operator

$$\vec{J} = \vec{L} + \tfrac{1}{2}\vec{\sigma} \tag{23}$$

commutes with the Hamiltonian. There is thus an SU(2) subgroup which accounts for 2j+1 of the degenerate states.

In addition, the "helicity" operator given above commutes with the Hamiltonian, and

$$\vec{\sigma}\cdot\vec{b}\;\Phi_{\nu K\mu} = S(K)\sqrt{E^2-m_0^2}\;\Phi_{\nu -K\mu} \tag{24}$$

If we define a set of operators

$$\chi_1 = \frac{1}{\sqrt{H^2-m_0^2}}\,\vec{\sigma}\cdot\vec{b}\;;\quad \chi_2 = i\chi_1\rho_3\frac{\vec{\sigma}\cdot\vec{L}+1}{|\vec{\sigma}\cdot\vec{L}+1|}\;;\quad \chi_3 = \rho_3\frac{\vec{\sigma}\cdot\vec{L}+1}{|\vec{\sigma}\cdot\vec{L}+1|} \tag{25}$$

we get a second SU(2) algebra

$$[X_k, X_\ell] = 2i\epsilon_{k\ell m} X_m \qquad \vec{X}\cdot\vec{X} = 3 \tag{26}$$

It is easy to see that this accounts for the degeneracy with respect to the sign of κ.

There still remains some degeneracy to be accounted for, and the next problem is to find the remaining operators. From the Lie algebra of the generators of the SO(4) group

$$[J_k, J_\ell] = i\epsilon_{k\ell m} J_m, \quad [J_k, M_\ell] = i\epsilon_{k\ell m} M_m; \quad [M_k, M_\ell] = i\epsilon_{k\ell m} J_m \tag{27}$$

we know that the operator which we seek should be a vector operator. By a vector operator we mean three operators satisfying the commutation relations

$$[J_k, A_\ell] = i\epsilon_{k\ell m} A_m \tag{28}$$

Analogously, a second rank tensor operator would be defined by

$$[J_k, A_{\ell m}] = i\epsilon_{k\ell n} A_{nm} + i\epsilon_{kmn} A_{\ell n} \tag{29}$$

The operator

$$\vec{\sigma} \times \vec{L}$$

is a pseudovector operator which changes the value of κ by one. For instance

$$(\vec{\sigma}\times\vec{L})_z \chi^{\mu}_{-\kappa} = -i\sqrt{(\ell+\mu-\tfrac{1}{2})(\ell-\mu-\tfrac{1}{2})}\,\chi^{\mu}_{\kappa-1} \tag{30}$$

for $j = \ell - \frac{1}{2}$, $\kappa = \ell$. However, it only changes the angular part of the wave function, and needs to be multiplied by an operator which changes the radial part. With the help of the ladder relations

$$\left[\frac{d}{dr} + \frac{\ell+1}{r} - \lambda^2 r\right] F_{\nu\ell} = 2\lambda\sqrt{\nu+1}\, F_{\nu+1,\ell-1}$$
$$\left[\frac{d}{dr} + \frac{\ell}{r} - \lambda^2 r\right] F_{\nu\ell} = -2\lambda\sqrt{\nu}\, F_{\nu-1,\ell+1} \qquad (31)$$

and the representation

$$\vec{\sigma}\cdot\vec{p} = -i\,\vec{\sigma}\cdot\hat{r}\left[\frac{d}{dr} + \frac{1}{r} - \frac{\vec{\sigma}\cdot\vec{L}+1}{r}\right] \qquad (32)$$

we introduce the operators

$$\vec{\Omega}^{+} = (\vec{\sigma}\times\vec{L})\vec{\sigma}\cdot\vec{a} \qquad \vec{\Omega} = \vec{\sigma}\cdot\vec{a}\,(\vec{\sigma}\times\vec{L}) \qquad (33)$$

where

$$\vec{\sigma}\cdot\vec{a} = \vec{\sigma}\cdot\vec{p} - i\lambda^2\,\vec{\sigma}\cdot\vec{r}\,\frac{\vec{\sigma}\cdot\vec{L}+1}{|\vec{\sigma}\cdot\vec{L}+1|}$$

Then either

$$\frac{1+\rho_3}{2}\vec{\Omega} + \frac{1-\rho_3}{2}\vec{\Omega}^{+} \qquad \text{or} \qquad \vec{\Omega} + \vec{\Omega}^{+}$$

is an invariant operator. When these operators act on the spinors $|\nu K\mu\rangle$, we obtain

$$\Omega_0^{+}|\nu K\mu\rangle = 2\lambda\sqrt{(\nu+1)(j-\mu)(j+\mu)}\,|\nu+1, K-1, \mu\rangle$$
$$\Omega_-^{+}|\nu K\mu\rangle = 2\lambda\sqrt{(\nu+1)(j-\mu)(j-\mu-1)}\,|\nu+1, K-1, \mu+1\rangle$$
$$\Omega_+^{+}|\nu K\mu\rangle = -2\lambda\sqrt{(\nu+1)(j+\mu)(j+\mu-1)}\,|\nu+1, K-1, \mu-1\rangle \qquad (34)$$

The matrix elements do not correspond to those of the irreducible representations of SO(4) given in Equation (45), Chapter II. Hence, it is not surprising that the commutation rules are not the same

$$\left[\Omega_k+\Omega_k^\dagger,\ \Omega_\ell+\Omega_\ell^\dagger\right] = -4i\lambda^2\epsilon_{k\ell m}J_m\left[H^2-m_o^2-3\lambda^2|K|\right] \tag{35}$$

Having realized this, it is a straightforward task to construct operators having the correct matrix elements, and hence the correct commutation relations. The result is

$$\begin{aligned}\vec{M} = &-i\frac{\sqrt{\frac{H^2-m^2}{4\lambda^2}+|K|-\frac{1}{2}}}{2\lambda(2|K|-1)}\ \frac{1}{2}\left[(\vec{\Omega}+\vec{\Omega}^\dagger)+\frac{K}{|K|}(\vec{\Omega}^\dagger-\vec{\Omega})\right]\\ &+\frac{1}{2}i\left[(\vec{\Omega}+\vec{\Omega}^\dagger)+\frac{K}{|K|}(\vec{\Omega}-\vec{\Omega}^\dagger)\right]\frac{\sqrt{\frac{H^2-m^2}{4\lambda^2}+|K|-\frac{1}{2}}}{2\lambda(2|K|-1)}\\ &-\frac{1}{2}\ \frac{H^2-m^2}{4\lambda^2(|K|-\frac{1}{2})(|K|+\frac{1}{2})}\vec{J}\end{aligned} \tag{36}$$

A check of the commutation rules then shows that

$$\begin{aligned}\left[M_k, M_\ell\right] &= i\epsilon_{k\ell m}J_m\\ \left[J_k, M_\ell\right] &= i\epsilon_{k\ell m}M_m\\ \left[X_k, M_\ell\right] &= 0\end{aligned} \tag{37}$$

We notice that the Lie algebra of SO(4) x SU(2) is realized and the invariants $\vec{M}$, $\vec{J}$, and X exhaust the degeneracy.

Now that the SO(4) x SU(2) invariance has been established, the question remains as to what happended to the SU(3) invariance group of the non-relativistic oscillator. Since the radial wave functions are the same we might expect the SU(3) group to survive. However, two points show that this argument is wrong. First, the non-relativistic limit of the Hamiltonian is (1)

$$H_{NR} = \frac{1}{2m_o}(p^2+\lambda^4r^2)+\frac{\lambda^2}{m_o}\left[(\vec{\sigma}\cdot\vec{L}+1)+\frac{1}{2}\right]\frac{\vec{\sigma}\cdot\vec{L}+1}{|\vec{\sigma}\cdot\vec{L}+1|} \tag{38}$$

Hence, there is a spin-orbit coupling which has shifted the energy levels. If we replace λ^2/m by the some number z, then there would be no degeneracy except that of the SU(2) group, 2j+1. In letting z go from zero to λ^2/m, we replace one "accidental" degeneracy by another. We cannot, in general, expect the group to be the same. The second point has to do with degeneracy also. The relativistic Hamiltonian possesses a degeneracy which is four times that of SU(3). In order to split the states of an energy level into four equal parts, we have to split up the SU(2) subgroup formed by the angular momentum operators. In doing this, we defeat the original purpose of the splitting.

It now remains to establish the non-invariance group for the problem. For this purpose, we follow the example set by Kiefer and Fradkin (7). We first show that the states with fixed sign of κ realize an irreducible representation of the group SO(4,1) and then give the non-invariance generators of this group. Strӧm has given the irreducible representations of SO(4,1) in the basis applicable here (31). The states with fixed sign of κ form a basis for the infinite dimensional irreducible representation $\pi^{+}_{\frac{1}{2},\frac{1}{2}}$ in the notation of Strӧm. This representation belongs to the discrete class, contrary to the cases discussed by Kiefer and Fradkin. To show this, we proceed as follows. The Casimir invariants of the SO(4) group are

$$C(1) = \frac{1}{2}\left(\vec{M}\cdot\vec{M}+\vec{J}\cdot\vec{J}\right) = \frac{1}{2}\left[\frac{(H^2-m^2)^2}{16\lambda^4} - \frac{3}{4}\right]$$
$$C(2) = \vec{J}\cdot\vec{M} = \frac{1}{2}\left[\frac{H^2-m^2}{4\lambda^2}\right] \qquad (39)$$

In the appropriate basis, we get the eigenvalues of the above invariant operators as

$$C(1) = \tfrac{1}{2}\left[(V+|K|+\tfrac{1}{2})^2 - \tfrac{3}{4}\right]$$
$$C(2) = \tfrac{1}{2}(V+|K|+\tfrac{1}{2}) \tag{40}$$

Following the discussion of Chapter II, we have

$$K^2 = \tfrac{1}{2}\left[C(1)+C(2)\right] = j_2(j_2+1)$$
$$L^2 = \tfrac{1}{2}\left[C(1)-C(2)\right] = j_1(j_1+1) \tag{41}$$

Hence, we find that

$$j_1 = \frac{v + |\kappa| - 1}{2}; \qquad j_2 = \frac{v + |\kappa|}{2} \tag{42}$$

and the dimensionalities ofthe SO(4) irreducible representations realized are

$$d' = (2j_1 + 1)(2j_2 + 1) = (n + 1)(n + 2) \tag{43}$$

where

$$n = v + |\kappa| - 1, \qquad n = 0,1,2,3,\ldots$$

Comparing Equations (43) and (22) we see that the doubling of states in d is due to the degeneracy in the sign of κ. The equivalence of the (j_1,j_2) parametrization to the irreducible representation $\pi^{+}_{r,q}$ of Strom is seen as follows. According to Strom, we have

$$\begin{aligned} r &= \min(j_1 + j_2) \\ q &= r, r-1, \ldots, \tfrac{1}{2} \\ n &= j_2 - j_1 \\ 1 &= j_1 + j_2 + 1 \end{aligned} \tag{44}$$

We therefore get

$$r = n = q = \tfrac{1}{2}$$
$$1 = v + |\kappa| + \tfrac{1}{2} \tag{45}$$

The allowed values of j_1 and j_2 are shown in Figure 2. This shows that the states with fixed sign of κ span an irreducible representation of SO(4,1).

We now proceed with the explicit construction of the relevant operators. In addition to the SO(4) generators, there exist also a scalar operator T and a vector operator $\vec{N}$ which obey the commutation relations of Equation (12).

For the irreducible representation of interest, the scalar operator T has the matrix elements specified by

$$T|v\,j\,\mu\rangle = \tfrac{1}{2}\sqrt{(v+2j+2)(v+1)}\,|v+1,j,\mu\rangle + \tfrac{1}{2}\sqrt{(v+2j+1)\,v}\,|v-1,j,\mu\rangle \tag{46}$$

This operator is represented for positive κ by

$$T = \frac{1}{4\lambda}\left[\sqrt{\frac{H^2-m_0^2}{4\lambda^2}+|K|-\tfrac{1}{2}}\;\frac{\vec{\sigma}\cdot\vec{b}}{\sqrt{H^2-m^2}}\,\vec{\sigma}\cdot\vec{a} + \vec{\sigma}\cdot\vec{a}\,\frac{\vec{\sigma}\cdot\vec{b}}{\sqrt{H^2-m^2}}\sqrt{\frac{H^2-m^2}{4\lambda^2}+|K|-\tfrac{1}{2}}\right] \tag{47}$$

The operator for the other sign of κ is given by interchanging

$$\frac{\vec{\sigma}\cdot\vec{b}}{\sqrt{H^2-m^2}} \quad \text{and} \quad \vec{\sigma}\cdot\vec{a}$$

The projection operators

$$\frac{1}{2}\left(1+\frac{\kappa}{|\kappa|}\right) \quad \text{and} \quad \frac{1}{2}\left(1-\frac{\kappa}{|\kappa|}\right)$$

then enable us to construct T in general. The vector operator $\vec{N}$ is then

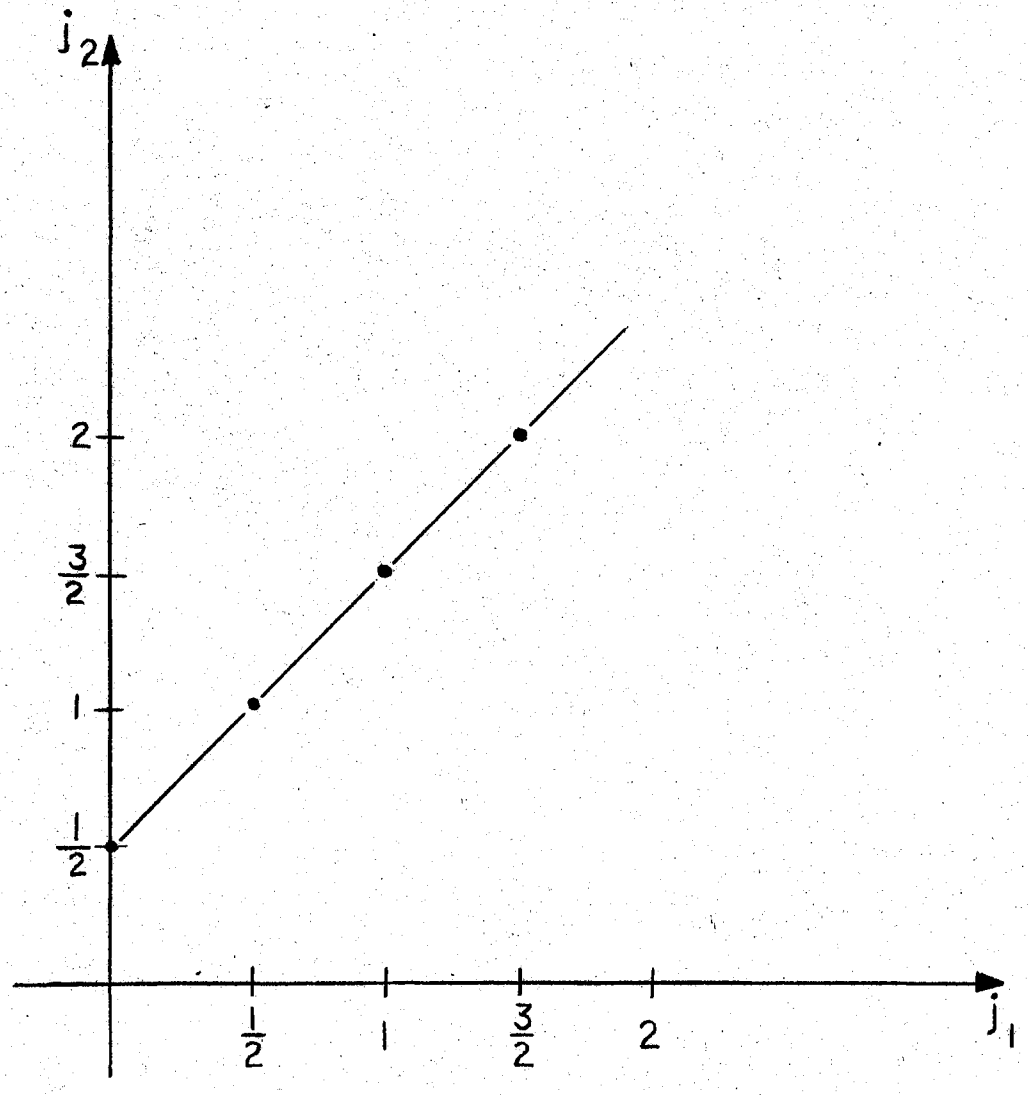

Figure 2. The Allowed Values of j_1 and j_2 Within the Irreducible Representation $\pi^{+}_{\frac{1}{2},\frac{1}{2}}$ of SO(4,1)

constructed by means of the relation

$$\vec{N} = -i[\vec{M},T] \tag{48}$$

This completes the set of SO(4,1) operators. The SU(2) operators $\vec{X}$ in Equation 25 are easily seen to commute with T, and hence with $\vec{N}$. Hence, all the operators of the SO(4,1) x SU(2) group have been realized.

CHAPTER IV

REVIEW OF COULOMB ENERGY CALCULATIONS

The Coulomb energies of nuclei have been under investigation since the mid-1930's. In the early days, Coulomb energies were used to estimate radii of mirror nuclei (isotopic spin $T = \frac{1}{2}$). The experimental energy difference between the nuclei of a mirror pair was taken from β decay data, or from the Q values of nuclear reactions. The models used then yielded the nuclear sizes necessary to obtain these differences in Coulomb energy. In modern times, however, there are more accurate methods for determining nuclear sizes. These include μ-mesonic atom X-ray data, and electron scattering data (Hofstadter (37)). Recently, the discovery of isobaric analog states in heavy nuclei has added another source of data (10), besides increasing the interest in Coulomb energy calculations. The calculations are so far in agreement with charge independence of nuclear forces (38), and the interest in Coulomb energies is based in part upon a desire to provide a more stringent test of this point. Other nuclear structure effects, such as the differences between neutron radii and proton radii, as well as the effects of deformations have also been studied (39).

In the present chapter, we review the methods of calculation that have been used, as well as the interpretations which have been given to the results. In the next chapter, the relativistic equivalent oscillator will be applied in an attempt to see what modifications of the Coulomb

energy originate from an assumed relativistic motion of nucleons.

The simplest model for calculating Coulomb energies is that of a uniformly charged sphere. This model was considered by Weizsacker (40) and Bethe (41). In this model, we suppose that the charge density due to a single proton is distributed uniformly inside a sphere of radius R. This gives the mutual electrostatic potential energy of one pair as

$$W = \frac{6}{5} \frac{e^2}{R} . \tag{1}$$

Since the total number of pairs of protons is $\frac{1}{2}Z(Z-1)$, then the total Coulomb energy is given by

$$E_c = \frac{3}{5} \frac{Z(Z-1)e^2}{R} . \tag{2}$$

If we next accept the saturation property of nuclear densities, i.e., that the volume of the sphere is proportional to the number of nucleons, we get

$$R = r_o A^{1/3} \tag{3}$$

and experimental data then tell us that $r_o = 1.2 \times 10^{-13}$ cm gives about the right Coulomb energy.

In order to make a quantum mechanical estimate, we use the Hartree approximation, writing the total nuclear wavefunction describing the notion of Z protons as a Slater determinant (in order to satisfy the Pauli principle). The Coulomb energy is then

$$E_c = \frac{1}{2} \sum_{i=1}^{Z} \sum_{j \neq i} \left[\int |\psi_i(\vec{r}_1)|^2 \frac{e^2}{r_{12}} |\psi_j(\vec{r}_2)|^2 d\vec{r}_1 d\vec{r}_2 - \int \psi_i^*(\vec{r}_1) \psi_j^*(\vec{r}_2) \frac{e^2}{r_{12}} \psi_i(\vec{r}_2) \psi_j(\vec{r}_1) d\vec{r}_1 d\vec{r}_2 \right] \tag{4}$$

We notice that the restriction $i \neq j$ on the sum can be dropped since those terms are zero. This corresponds to adding self energy terms to the first part, called the direct energy, and adding the negative of these self energy terms to the second part, called the exchange energy.

Probably the first estimate of these direct and exchange energies was made by Flugge (42). His direct energy (not including self energy) was

$$E_c = \frac{1}{\sqrt{\pi}} \frac{Z(Z-1)e^2}{R} \tag{5}$$

and was obtained by assuming angle-independent single particle wave functions of the form

$$\psi(r) = A\, e^{-r^2/R^2} \tag{6}$$

where

$$A^2 = \left(\frac{2}{\pi}\right)^{3/2} \frac{Z}{R^3} \tag{7}$$

His evaluation of the exchange energy, however, was erroneous, resulting in zero total Coulomb energy for Helium nuclei.

Bethe (44) evaluated the direct and exchange energies using the statistical model. In this model, the single particle wavefunctions are taken as plane waves inside the nucleus, and zero outside corresponding to motion inside a constant square well with rigid walls. The boundary condition on the surface restricts the values of the particle momentum, and in addition, a maximum allowed momentum is imposed consistent with the total number of occupied states. If we define ordinary and mixed

densities by the equations

$$\rho_p(\vec{r}) = \sum_{i=1}^{Z} |\psi_i(\vec{r})|^2 \tag{8}$$

$$\rho_p(\vec{r}_1, \vec{r}_2) = \sum_{i=1}^{Z} \psi_i^*(\vec{r}_1)\psi_i(\vec{r}_2) \tag{9}$$

then, if we have an even Z nucleus, and average over the spins, we get

$$E_c = \frac{1}{2}\int \frac{e^2}{r_{12}} \rho_p(\vec{r}_1)\rho_p(\vec{r}_2) d\vec{r}_1 d\vec{r}_2 - \frac{1}{4}\int \frac{e^2}{r_{12}} |\rho_p(\vec{r}_1, \vec{r}_2)|^2 d\vec{r}_1 d\vec{r}_2$$

Bethe evaluated the exchange density by approximating the sum in Equation (9) by an integral, with the result

$$\rho_p(\vec{r}_1, \vec{r}_2) = \frac{\sin k_o r_{12} - k_o r_{12} \cos k_o r_{12}}{\pi^2 r_{12}^3} \tag{10}$$

Bethe then obtains the Coulomb energy as

$$E_c = \frac{e^2}{r_o A^{1/3}} (0.600\ Z^2 - 0.460\ Z^{4/3}) \tag{11}$$

Much later, Sengupta (43) pointed out that there is an error in the above derivation if Z is odd (resulting from an unpaired spin). The correct equation is then

$$E_c = \frac{e^2}{R} [0.60\ Z^2 - 0.46\ Z^{4/3} - [1-(-1)^Z]0.15] \tag{12}$$

In 1938, Bethe calculated the Coulomb energies of light nuclei (44), in which the last nucleon's wavefunction was allowed to extend beyond

the radius of the residual nucleus

$$\psi(r) = \frac{\alpha}{R} \qquad r < R$$
$$\psi(r) = \frac{\alpha}{r} e^{-(r-R)/b} \qquad r > R \tag{13}$$

The constant b was estimated using experimentally measured binding energies. Alternatively, by using the results of the statistical model for the Coulomb energy, the binding energies of unknown nuclei was estimated. Bethe thus was able to draw conclusions about the stability of unknown nuclei, and he pointed out that this had applications in astrophysics.

Following the supermultiplet theory of Wigner using LS coupling (45), Feenberg and Goertzel (46), tried to study the variation of Coulomb energies from even Z to odd Z nuclei. By assuming that nuclear forces were not strongly spin dependent, they were able to demonstrate the importance of a "pairing effect". This effect is due to the fact that nuclear forces are short ranged, and favor paired spins, so that the total proton spin S is ½ for odd Z nuclei and zero for even Z nuclei. The Pauli principle then causes a larger probability for two protons to be close together if they have paired spins, and hence a symmetric spatial wave function. In quantitative terms, Feenberg and Goertzel showed that the Coulomb energy expression is of the form

$$E_c = \frac{1}{2} Z(Z-1)\ L_c + \frac{3}{8} (Z-\tfrac{1}{2} + \tfrac{1}{2}\ (-1)^Z) L_c' \tag{14}$$

In the late 1940's and early 1950's, various calculations were made using finite and infinite square wells, and diffuse boundary potentials. Cooper and Henley (47) attempted to explain the small radii, r_o = 1.20

fermis, of light nuclei which had been found by extrapolation from μ-mesonic atom experiments. Jancovici (48), calculated the Coulomb energy differences of the $O^{17} - F^{17}$ and $O^{15} - N^{15}$ pairs and showed that the radii needed to match the experimental differences were in serious disagreement with mirror nuclei data. It was later pointed out by Sood and Green (49) that the discrepancies were not so bad, since electron scattering data gave larger radii, $r_o = 1.30$, for light nuclei than the μ-mesonic X-ray data.

Calculations based on an infinite oscillator well and jj coupling were carried out by Carlson and Talmi (50). Their calculations showed a pairing effect in mirror nuclei, similar to that considered by Feenberg and Goertzel. However, they used jj coupling, and took correlations into account, that is, they assumed that proton seniority was a good quantum number. The seniority, introduced by Racah (51), is an additional quantum number used to label many particle wave functions. If we consider a configuration j^n of n equivalent particles, the seniority is the smallest number of particles, v, which possess a state transforming under the group Sp(2j+1) exactly like the state for the n particles. Here Sp(2j+1) is the symplectic group in 2j+1 dimensions, which is the group which leaves invariant a bilinear antisymmetric form of two vectors (52). The Carlson and Talmi assumption of lowest proton seniority then amounts to assuming that the total angular momentum of the protons in the j^2 configuration is J = 0 (seniority v = 0) and J = j for the j^3 configuration (seniority v = 1). For nuclei, in which the forces are short ranged, this happens to be a reasonable assumption, whereas in atomic physics it would not be reasonable. The application of the above theory leads to the expression for the contribution of the j^n configura-

tion to the interaction as

$$E_c(j^n) = \frac{n(n-1)}{2}\left(\frac{2(j+1)\,\bar{V}_2 - V_o}{2j+1}\right) + \left[\frac{n}{2}\right]\frac{2(j+1)}{2j+1}\,(V_o - \bar{V}_2) \qquad (15)$$

Here $\bar{V}_2$ and V_o are given in terms of Slater integrals (23), and $\left[\frac{n}{2}\right]$ stands for the largest integer not exceeding n/2. There is a pairing effect since the above expression depends on whether n is even or odd.

Carlson and Talmi evaluated the Coulomb energy differences between mirror nuclei using the above theory. For light nuclei, they found that the radius parameter r_o needed to match the experimental Coulomb energy was too large compared to the experimental values. This discrepancy persists even today, as has been discussed by Goldhammer (53), who concluded that $r_o = 1.25$ is the best experimental value for light nuclei.

For Helium, the effect of the hard core potential of nucleons has been used to get agreement, as has been discussed by Ohmura et. al. (54).

On the other hand, the correction for the center of mass motion of the nucleus is also of importance, and has been used by Wilkinson (38) in his studies of the 1p shell. This effect enters through the determination of the oscillator constant λ which appears in the oscillator Hamiltonian. It is customary to determine this parameter by the "equivalent uniform radius" criterion. In this method, the equivalent uniform radius is defined as the radius of a uniform spherical mass distribution having the same expectation value of r^2 as the shell model result. This leads to the result (Elton (55))

$$R = \left[\frac{5}{3A}\,\Sigma\,\langle r^2\rangle\right]^{1/2} = r_o\,A^{1/3} \qquad (16)$$

where the sum is over all nucleons. If the center of mass is in its lowest allowed state, then the correction for its motion amounts to the substitution (Elliott and Skyrme (56))

$$\langle r^2 \rangle \rightarrow \langle r^2 \rangle - \frac{3}{2A} \frac{1}{\lambda^2} \tag{17}$$

For light nuclei, this correction happens to bring the calculations into better agreement with experiment. For A > 20, it is negligible.

In an attempt to obtain better estimates of the contributions of the direct and exchange Coulomb energies to Weizsacker nuclear mass formula, Green and Swamy (57), calculated the total Coulomb energies of light nuclei. Both oscillator potential and diffuse boundary potentials were used. As a follow up to this work, Swamy, Kembhavi, and Galgali (58) used oscillator wave functions to calculate the Coulomb energies of closed shell nuclei in the medium to heavy mass range. Comparing calculations with the statistical model and the trapezoidal model of Cameron (59), they found that the direct energies were model independent, for practical purposes. However, the exchange energies were model dependent. The $Z^{4/3}$ variation of Bethe's statistical model agrees with the results of the oscillator calculation, but the coefficients are different.

The Coulomb energy terms in the Weizacker mass formula have also been studied by Mozer (60). The direct and exchange terms were considered, as well as the effects of nuclear deformations. Numerous authors have used the Bohr-Wheeler liquid drop model to study this deformation effect (61, 62).

Returning to the subject of mirror nuclei, there have been calculations by Unna and Unna et. al. (63, 64) which have tested Carlson and

Talmi's assumption of lowest proton seniority. Since some nuclei have neutrons as well as protons outside closed shells, it is conceivable that they might cause proton seniority to be a poor quantum number. Unna's calculations were less approximate, since they considered isospin and combined neutron-proton seniority to be good quantum numbers. The results showed that Carlson and Talmi's calculations were not appreciably modified, the differences being less than 1% in all cases. In addition, for nuclei with $29 < A < 64$, it was shown that calculations using harmonic oscillator wave functions are capable of yielding close quantitative agreement with the experimental results.

It should be noted, however, that configuration mixing becomes more important in heavy nuclei. For instance, studies of the Hartree-Fock approximation (65) have shown that occupied states of Pb^{208} are appreciably different from pure oscillator functions.

Besides these oscillator calculations, there have been attempts to use the real part of the Woods-Saxon potential (66)

$$V(r) = \frac{V_o}{e^{\left(\frac{r-R}{a}\right)} + 1} \tag{18}$$

A charge distribution $\rho_p(r)$ giving an electrostatic potential is also assumed, and the wave functions are generated by putting these potentials into the Schroedinger equation. The problem cannot be solved analytically, and requires the use of a computer.

Calculations using this technique have been reported by Wilkinson, et. al. (38), and by Nolen, Schiffer, et. al. (67). They calculated Coulomb energy differences between isobaric analog states.

In the version of Nolen, Schiffer, et. al., which was applied to

medium and heavy nuclei, one of the excess neutrons of a state is replaced by a proton to give the analog state. In other words, the proton is assumed to have the same density distribution as the neutron excess. The direct integrals contribute to the Coulomb energy difference the amount

$$\Delta E_c = 4\pi e \int_0^\infty \rho_{ne}(r)\, V(r)\, r^2 dr \tag{19}$$

where

$$V(r) = \int_\infty^r \frac{4\pi Ze}{r'^2}\left[\int_0^{r'} \rho_p(r'')\, r''^2 dr''\right] dr' \tag{20}$$

and

$$\rho_{ne}(r) \equiv \rho_n(r) - \rho_p(r) \tag{21}$$

The exchange term is evaluated independently using the wave functions. In addition, a spin-orbit term, which arises partly from the Thomas precession and partly from the difference between the neutron and proton magnetic moments, is included.

The results show close agreement with experiment provided the parameters in the charge distribution are allowed to vary within the limits allowed by the experimentally measured binding energy and expectation value of r^2. For instance, in Pb^{208} the Coulomb energy difference can be adjusted to 18.980 MEV, in agreement with experiment. Conclusions are drawn concerning the radius of the neutron excess as compared to the radius of the nucleus as a whole. In addition, studies are made of the shift of the nuclear radius from isotope to isotope, such as in the series Ca^{40} to Ca^{49}.

CHAPTER V

APPROXIMATE, RELATIVISTIC COULOMB ENERGY CALCULATIONS

In reviewing Coulomb energy calculations (Chapter IV), we found no calculations which have attempted to correct for relativistic motion of nucleons. This was probably due to the conclusion of most investigators that non-relativistic calculations agree close enough with experiment. Twenty or thirty years ago, various relativistic calculations were made of the binding energies of light nuclei, such as the deuteron, triton, or alpha particle. Blochinzew (68) and Margenau (69) applied the Klein-Gordan equation to a study of the deuteron binding energy. In 1936, Feenberg (70) looked at relativistic corrections to the deuteron kinetic energy, which led to a 25% change of the kinetic energy predicted by the non-relativistic, single particle theory. Primakoff (71), Breit (72), Siegel (73), and Blatt and Weisskopf (74) have noted that relativistic corrections to magnetic moment and binding energy calculations are not entirely negligible. There thus seems to be a need for estimating the magnitude of the relativistic corrections to the Coulomb energies. We therefore turn to the relativistic equivalent oscillator, and the predictions of the approximate, relativistic shell model of Braun and Swamy (32).

For the normalized, single particle wave functions, we take

$$\Phi_{\nu K\mu} = \begin{bmatrix} \sqrt{\frac{E+m_0c^2}{2E}}\,|\nu K\mu\rangle \\ S(K)\sqrt{\frac{E-m_0c^2}{2E}}\,|\nu K\mu\rangle \end{bmatrix} \tag{1}$$

with the various quantities in this equation defined as in Chapter III.

For closed shell nuclei, or nuclei with one particle outside a closed shell, the shell model wavefunctions (with lowest proton seniority) are given by a single Slater determinant. In other cases, because of coupling and many body effects, a more complicated linear combination of Slater determinants is necessary. The expectation value of Coulomb energy is then evaluated using Racah algebra, as in the book by Talmi and de Shalit (52). In this jj coupling model, the Coulomb energy due to the interaction of the $2j\pm1$ particles in the j shell with the $2j'+1$ particles in the j' shell is

$$E_c(jj') = \tfrac{1}{2}(2j+1)(2j'+1)\Big[\frac{E+m_0c^2}{2E}\,\frac{E'+m_0c^2}{2E'}\,F^0(\nu\ell;\nu'\ell')$$
$$+\frac{E-m_0c^2}{2E}\,\frac{E'+m_0c^2}{2E'}\,F^0(\nu\bar{\ell};\nu'\ell') + \frac{E+m_0c^2}{2E'}\,\frac{E'-m_0c^2}{2E'}\,F^0(\nu\ell;\nu'\bar{\ell}')$$
$$+\frac{E-m_0c^2}{2E}\,\frac{E'-m_0c^2}{2E'}\,F^0(\nu\bar{\ell};\nu'\bar{\ell}')\Big]$$
$$-\tfrac{1}{2}(2j'+1)\sum_k \left|C^{j'\,k\,j}_{\ell\,-\frac{1}{2}\;0\;-\frac{1}{2}}\right|^2 \frac{1+(-1)^{\ell+\ell'+k}}{2}\;\times$$
$$\times\Big[\frac{E+m_0c^2}{2E}\,\frac{E'+m_0c^2}{2E'}\,G^k(\nu\ell;\nu'\ell') \;+$$

$$+\sqrt{\frac{(E^2-m_0^2c^4)(E'^2-m_0^2c^4)}{16\,E^2E'^2}}\;S(K)S(K')\,R^k(v\ell,v\bar{\ell};v'\ell',v'\bar{\ell}')$$

$$+\sqrt{\frac{(E^2-m_0^2c^4)(E'^2-m_0^2c^4)}{16\,E^2E'^2}}\;S(K)S(K')\,R^k(v\bar{\ell},v\ell;v'\bar{\ell}',v\ell')$$

$$+\frac{E-m_0c^2}{2E}\,\frac{E'-m_0c^2}{2E'}\,G^k(v\bar{\ell};v'\bar{\ell}')\Bigg] \tag{2}$$

Here the F^0, G^k, and R^k are Slater integrals, in the notation of Condon and Shortley (23). In the non-relativistic limit, the energy of a particle is approximately equal to its rest energy, and this reduces to

$$E_c(jj') = \tfrac{1}{2}(2j+1)(2j'+1)\,F^0(v\ell;v'\ell')$$
$$-\tfrac{1}{2}(2j'+1)\sum_k \begin{pmatrix} j' & k & j \\ -\frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}^2 \frac{1+(-1)^{\ell+\ell'+k}}{2}\,G^k(v\ell;v'\ell') \tag{3}$$

The Slater integral F^k is given by

$$F^k(v_1\ell_1;v_2\ell_2) = e^2\int_0^\infty\int_0^{r_2} |F_{v_1\ell_1}(r_1)|^2\,\frac{r_1^k}{r_2^{k+1}}\,|F_{v_2\ell_2}(r_2)|^2\,r_1^2r_2^2\,dr_1\,dr_2$$
$$+e^2\int_0^\infty\int_0^{r_2} |F_{v_1\ell_1}(r_1)|^2\,\frac{r_2^k}{r_1^{k+1}}\,|F_{v_2\ell_2}(r_2)|^2\,r_1^2r_2^2\,dr_1\,dr_2 \tag{4}$$

where the $F_{v\ell}$'s are the radial solutions

$$F_{v\ell}(r) = \lambda\,N_{v\ell}\,(\lambda r)^\ell\,e^{-\frac{1}{2}(\lambda r)^2}\,{}_1F_1(-v,\ell+\tfrac{3}{2};(\lambda r)^2) \tag{5}$$

To evaluate this expression we use the identity

$${}_1F_1(-v_1,\ell_1+\tfrac{3}{2};(\lambda r)^2)\,{}_1F_1(-v_2,\ell_2+\tfrac{3}{2};(\lambda r)^2) =$$

$$= \sum_{n=0}^{V_1+V_2} \left[\sum_{k=0}^{n} \frac{(-V_1)_k \, (-V_2)_{n-k}}{k!\,(n-k)!\,(\ell_1+\frac{3}{2})_k \,(\ell_2+\frac{3}{2})_{n-k}} \right] (\lambda r)^{2n} \tag{6}$$

From this we obtain, using the abbreviation

$$A(V_1 V_2 \ell_1 \ell_2 n) = \sum_{k=0}^{n} \frac{(-V_1)_k \, (-V_2)_{n-k}}{k!\,(n-k)!\,(\ell_1+\frac{3}{2})_k \,(\ell_2+\frac{3}{2})_{n-k}} \tag{7}$$

the result

$$F^k(V_1 \ell_1 ; V_2 \ell_2) = \frac{1}{\lambda} (N_{V_1 \ell_1} N_{V_2 \ell_2})^2 \sum_{n=0}^{2V_1} \sum_{m=0}^{2V_2} A(V_1 V_1 \ell_1 \ell_1 n) \times$$

$$\times A(V_2 V_2 \ell_2 \ell_2 m) \left[\frac{1}{2\ell_1+2n+k+3} \int_0^\infty u_2^{2(\ell_1+\ell_2+n+m+2)} e^{-2u_2^2} \, {}_1F_1(1; \ell_1+n+\tfrac{k+5}{2}; u_2^2) \, du_2 \right.$$

$$\left. + \frac{1}{2\ell_2+2m+k+3} \int_0^\infty u_1^{2(\ell_1+\ell_2+m+n+2)} e^{-2u_1^2} \, {}_1F_1(1; \ell_2+m+\tfrac{k+5}{2}; u_1^2) \, du_1 \right] \tag{8}$$

Using the formula (75)

$$\int_0^\infty e^{-st} t^{b-1} \, {}_1F_1(a, c; kt) = \Gamma(b)(s-k)^{-b} \, {}_2F_1(c-a, b, c; \frac{k}{k-s}) \tag{9}$$

we get

$$F^k(V_1 \ell_1 ; V_2 \ell_2) = \frac{e^2}{4\lambda^2} (N_{V_1 \ell_1} N_{V_2 \ell_2})^2 \sum_{n=0}^{2V_1} \sum_{m=0}^{2V_2} A(V_1 V_1 \ell_1 \ell_1 n) \times$$

$$\times A(V_2 V_2 \ell_2 \ell_2 m) \, \frac{\Gamma(\ell_1+\ell_2+n+m+\frac{5}{2})}{2^{\ell_1+\ell_2+n+m+5/2}} \times$$

$$\times \left[\frac{1}{l_1+n+\frac{k+3}{2}} \, {}_2F_1\left(l_1+l_2+n+m+\tfrac{5}{2}; 1; l_1+n+\tfrac{k+5}{2}; \tfrac{1}{2}\right) \right.$$

$$\left. + \frac{1}{l_2+m+\frac{k+3}{2}} \, {}_2F_1\left(l_1+l_2+n+m+\tfrac{5}{2}; 1; l_2+m+\tfrac{k+5}{2}; \tfrac{1}{2}\right) \right] \tag{10}$$

We have been using the normalization factor

$$N_{ve} = \left[\frac{2\lambda}{v!} \frac{\Gamma(v+l+3/2)}{\left[\Gamma(l+3/2)\right]^2} \right]^{1/2} \tag{11}$$

It is apparent that the Slater integrals are directly proportional to $e^2\lambda$.

The other Slater integrals G^k and R^k can be evaluated by the same method, the result of which is suitable for computer programming. These results were originally given by Swamy, Kembhavi, and Galgali (58).

In order to use these equations to calculate the Coulomb energy of a nucleus, we have to assign values of v, κ, and μ to the states of the particles. These assignments must be consistent with experimentally measured spins and parities of nuclei, and this can be done by using the quantum numbers v, κ, and j which have been used in the non-relativistic shell model.

Next, the oscillator constant λ must be determined. This is accomplished by using the usual equivalent uniform radius criterion (Chapter IV).

$$\left[\frac{5}{3A} \Sigma \langle r^2 \rangle\right]^{1/2} = r_o A^{1/3} \tag{12}$$

The values of r_o are taken either from electron scattering data (37), or alternatively, adjusted to match the experimentally measured Coulomb energy differences. If ψ_A is the antisymmetric determinantal proton wavefunction, then

$$\int \psi_A^\dagger r_1^2 \psi_A \, d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_Z = \frac{1}{Z} \sum_{\nu k \mu} \langle r^2 \rangle_{\nu k \mu} \tag{13}$$

If r_1 were a neutron coordinate, we would get instead

$$\frac{1}{N} \sum_{\nu k \mu} \langle r^2 \rangle_{\nu k \mu} \tag{14}$$

Hence

$$\frac{1}{A} \sum_{i=1}^{A} \langle r_i^2 \rangle = \frac{1}{A} \left[Z \cdot \frac{1}{Z} \sum_{\substack{\nu k \mu \\ \text{protons}}} \langle r^2 \rangle_{\nu k \mu} + N \cdot \frac{1}{N} \sum_{\substack{\nu k \mu \\ \text{neutrons}}} \langle r^2 \rangle_{\nu k \mu} \right] \tag{15}$$

$$= \frac{1}{A} \sum_{\nu k \mu} \langle r^2 \rangle_{\nu k \mu}$$

where the final sum applies to the quantum numbers of all the nucleons. This shows that the sum is replaceable by a sum over single particle matrix elements. Putting this in the relativistic single particle wave functions then gives

$$\langle r^2 \rangle_{\nu k \mu} = \frac{1}{\lambda^2} \left[(2\nu + \ell + \tfrac{3}{2}) + (\bar{\ell} - \ell) \frac{E - m_0 c^2}{2E} \right] \tag{16}$$

where

$$\bar{\ell} = \ell + 1 \quad \text{for} \quad j = \ell + \tfrac{1}{2}, \; K < 0$$

$$\bar{\ell} = \ell - 1 \quad \text{for} \quad j = \ell - \tfrac{1}{2}, \; K > 0$$

$$E = \sqrt{m_0^2 c^4 + 4\lambda^2 (\hbar c)^2 (\nu + |K| + \tfrac{1}{2})^2}$$

We notice that if we have a closed shell in the sense of the exact equivalent oscillator, then the number of single particle wavefunctions with $\kappa > 0$ equals the number with $\kappa < 0$, and the expression gives the same result as

$$\langle r^2 \rangle_{V\kappa\mu} = \frac{1}{\lambda^2}\left(2V + \ell + \frac{3}{2}\right) \tag{17}$$

which is the non-relativistic result. Hence, the value of λ determined by this method would be the same. However, as we go toward heavier nuclei, studies show that the $\kappa < 0$ levels are filled before the $\kappa > 0$ levels. For instance, the $1d_{5/2}$ levels are filled before the $2s_{1/2}$, but the $1f_{5/2}$ levels are usually filled afterwards. Hence, in practice there is a relativistic correction to λ even for closed shell nuclei.

The above methods were used to calculate Coulomb energies. Tables of results and the computer program are given in Appendices A and B.

For the non-relativistic calculations, when we divide the total Coulomb energy by $e^2\lambda$, we have a quantity which is independent of λ. However, in the relativistic case, there remains a slight, second order dependence on λ due to the dependence of E on λ. As we go to heavier nuclei, the general trend is for the differences in the non-relativistic and relativistic direct Coulomb energies divided by $e^2\lambda$ to increase according to

$$\left.\frac{E_{DIRECT}}{e^2\lambda}\right|_{REL.} - \left.\frac{E_{DIRECT}}{e^2\lambda}\right|_{\substack{NON-\\REL.}} = -0.0093A \tag{18}$$

However, when λ is calculated relativistically, the non-relativistic

Coulomb energy becomes more nearly equal to the relativistically calculated value. Whether it is smaller or larger generally depends on the nucleus and the value of r_o.

Since the differences in the relativistic and non-relativistic Coulomb energies happen to be usually less than 1% as can be seen from the tables in Appendix A, it appears that the neglect of relativistic corrections by earlier workers is justified, at least for medium sized nuclei.

In the excited states of nuclei, it is conceivable that the kinetic energy of a nucleon might become abnormally large. However, the shell model becomes less valid for these states, generally as the energy increases, which can be explained as due to configuration mixing. Calculations were made for the first excited states of F^{19} and Sc^{41}. The results show the usual 1% differences.

In light nuclei, center of mass motion is an important correction to consider (see Chapter IV). Relativistically, it is the center of momentum and not the center of mass which is well defined. However, Bethe and Salpeter (75) have shown that, in the two particle problem, a substitution of the reduced mass into the Dirac equation yields the first approximation. It therefore seems permissible to use the non-relativistic approximation for this correction in the relativistic expression. This means the substitution

$$\langle r^2 \rangle \rightarrow \langle r^2 \rangle - \frac{3}{2A\lambda^2} \tag{19}$$

in the equation for determining λ. It is found that this substitution enables the $_2He^3$ coulomb energy to be placed in better agreement with

experiment. This also applies to the $_7N^{13}$ -- $_6C^{13}$ Coulomb energy difference. In addition, the difference between relativistic and non-relativistic calculations becomes larger, but is still less than 2%.

The largest relativistic corrections occur for heavy nuclei. For lead, the direct energy differs by 1%, but the exchange energies differ by a comparatively large 3%. It may be significant to note that 3% happens to be 1 MEV in this case. It is also interesting to note that these simple non-relativistic and relativistic models, with $r_o = 1.20$ fermis, give good agreement with experiment. The relativistic and non-relativistic Coulomb energy differences between Pb^{208} and its analog state are found to be 19.4 MEV and 19.3 MEV, respectively, in agreement with the experimental value 18.980 MEV. By adjusting r_o slightly we could obtain exact agreement.

CHAPTER VI

CONCLUSIONS

In the first part of this work, we were able to draw some conclusions concerning the group structure of the relativistic equivalent oscillator. These results add to the knowledge of group theory as related to relativistic quantum mechanics. It has already been mentioned that such knowledge happens to be useful in elementary particle physics, where the interactions are not explicitly known and the equations not established. In the second part, we applied the shell model of Braun and Swamy (32), which is based upon the relativistic equivalent oscillator, to the study of Coulomb energies. It has been shown that relativistic corrections are small, but are most important in heavy nuclei.

In the last part of Chapter III, the solutions of the relativistic equivalent oscillator Hamiltonian were shown to provide a basis for one infinite dimensional irreducible representation, $\pi^{+}_{\frac{1}{2},\frac{1}{2}}$, of the group SO(4,1) x SU(2). Operators corresponding to the Lie algebra of this group have been given. These operators convert a wavefunction corresponding to one energy level into one corresponding to another.

It was also shown that SO(4) x SU(2) is an invariance group of the same Hamiltonian. This meant that there exist certain irreducible representations under which the wavefunctions corresponding to a given energy level are transformed among themselves. The irreducible representations of SO(4) were derived in Chapter II from the commutation re-

lations, the Casimir invariants, and the requirement that the operators which represent the Lie generators be Hermitian. Hence, the energy spectrum may be derived from these requirements.

Our simple shell model, based upon the relativistic equivalent oscillator, gives results which are almost identical with the non-relativistic shell model results. Both models give exchange and direct energies which vary only locally from the Z,A dependence found by Bethe from the statistical model (41). In addition, a small pairing effect can be seen in a graph of exchange energy versus $Z^{4/3}/A^{1/3}$.

The relativistic corrections become largest for lead, where the relativistic exchange energy is found to be about 1 MEV less than the non-relativistic, which may be interpreted as meaning that the nucleons in more tightly bound nuclei may move with relativistic speeds.

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APPENDIX A

Tables showing the results of the Coulomb energy calculations of the present work are given. The symbol CM beside the name of a nucleus means that the correction for center of mass motion is included. The Slater integrals were evaluated by computer, but exact expressions for the first few of these quantities were found and checked with the results of the computer analysis. These Slater integrals are given here in separate tables.

TABLE I

COULOMB ENERGIES DIVIDED BY $e^2\lambda$

Element	Non-relativistic		r_o	Relativistic	
	Direct	Exchange		Direct	Exchange
He^3	1.5976	0.79788	1.33	1.57432	0.78716
He^4	1.5976	0.79788	1.20	1.57400	0.78700
C^{13}	11.702	2.660	1.20	11.597	2.636
			1.28	11.608	2.638
N^{13}	15.426	2.926	1.20	15.321	2.871
			1.28	15.332	2.877
O^{17}	20.346	3.790	1.29	20.270	3.725
$O^{17}(2s_{1/2})$	20.346	3.790	1.29	20.270	3.725
F^{17}	24.721	4.036	1.29	24.619	3.966
$F^{17}(2s_{1/2})$	24.901	4.006	1.29	24.804	3.935
Ca^{40}	109.355	10.784	1.22	109.084	10.576
Ca^{41}	109.335	10.784	1.18	109.070	10.564
Ca^{49}	109.335	10.784	1.24	109.101	10.590
Sc^{41}	118.850	11.128	1.18	118.538	10.913
Sc^{49}	119.196	11.092	1.24	118.930	10.890
Pb^{208}	1442.68	54.610	1.20	1440.71	52.907
$(Bi^{208})^*$	1475.50	55.079	1.20	1473.55	53.356

TABLE II

COULOMB ENERGIES IN MEV

Element	Non-relativistic		r_o fermis	Relativistic	
	Direct	Exchange		Direct	Exchange
He^3	1.8940	0.9470	1.33	1.8938	0.9469
He^3(CM)	1.5464	0.7732	1.33	1.5535	0.7767
He^4	1.9069	0.9534	1.20	1.9095	0.9547
C^{13}	10.702	2.432	1.28	10.689	2.429
C^{13}(CM)	10.416	2.367	1.28	10.408	2.366
N^{13}	14.107	2.675	1.28	14.118	2.649
N^{13}(CM)	13.731	2.604	1.28	13.746	2.590
O^{17}	17.381	3.238	1.29	17.389	3.196
$O^{17}(2s_{1/2})$	17.381	3.238	1.29	17.385	3.195
F^{17}	21.119	3.448	1.29	21.119	3.402
$F^{17}(2s_{1/2})$	21.272	3.422	1.29	21.274	3.375
Ca^{40}	84.372	8.322	1.22	84.282	8.171
Ca^{41}	87.043	8.585	1.18	86.959	8.422
Ca^{49}	81.066	7.996	1.24	81.063	7.868
Sc^{41}	94.618	8.859	1.18	94.508	8.690
Sc^{49}	88.378	8.224	1.24	88.366	8.091
Pb^{208}	861.856	32.624	1.20	861.788	31.647
(Bi^{208})*	881.465	32.904	1.20	881.433	31.916

TABLE III

THEORETICAL AND EXPERIMENTAL COULOMB DISPLACEMENT ENERGIES IN MEV

PAIR	STATE	r_o fermis	ΔE_c non-rel.	$e^2\lambda$ non-rel.	ΔE_c rel.	$e^2\lambda$ rel.	ΔE_c exp.
He^3-H^3	ground	1.33	0.773	0.969	0.777	0.983	0.76
(CM)		1.20	0.857	1.074	0.862	1.092	
He^3-H^3	ground	1.20	1.0496	1.315	1.049	1.337	
N^{13}-C^{13}	ground	1.28	3.078	0.890	3.123	0.896	3.003
(CM)		1.20	3.283	0.950	3.337	0.957	
N^{13}-C^{13}	ground	1.20	3.373	0.975	3.387	0.983	
F^{17}-O^{17}	ground	1.29	3.527	0.854	3.524	0.858	3.545
	$2s_{1/2}$	1.29	3.706	0.854	3.710	0.858	3.174
Ca^{41}-Sc^{41}	ground	1.18	7.300	0.796	7.281	0.797	7.28
	ground	1.22	7.060	0.770	7.043	0.771	
	$2p_{3/2}$	1.18	7.606	0.796	7.594	0.797	6.99
Ca^{49}-Sc^{49}	ground	1.24	7.083	0.741	7.080	0.743	7.09
		1.18	7.444	0.779	7.439	0.781	
$(Bi^{208})^*$ -Pb^{208}	analog and ground	1.20	19.329	0.597	19.376	0.598	18.980

TABLE IV

EXACT EXPRESSIONS FOR THE SLATER INTEGRALS

$F^{o}(v1;v'1')$ DIVIDED BY $e^{2}\lambda\sqrt{\frac{2}{\pi}}$

	1s	1p	1d	1f	2s
1s	1	$\frac{5}{6}$	$\frac{43}{60}$	$\frac{177}{280}$	$\frac{19}{24}$
1p		$\frac{3}{4}$	$\frac{27}{40}$	$\frac{1027}{1680}$	$\frac{11}{16}$
1d			$\frac{151}{240}$	$\frac{1963}{3360}$	$\frac{299}{480}$
1f				$\frac{1241}{2240}$	$\frac{3863}{6720}$
2s					$\frac{131}{192}$

TABLE V

EXACT EXPRESSIONS FOR THE SLATER INTEGRALS

$G^k(v1;v'1')$ DIVIDED BY $e^2\lambda\sqrt{\frac{2}{\pi}}$

	k	1s	k	1p	k	1d	k	1f	k	2s
1s	0	1	0	$\frac{1}{2}$	0	$\frac{1}{4}$	0	$\frac{1}{8}$	0	$\frac{1}{8}$
1p			0	$\frac{3}{4}$	1	$\frac{11}{24}$	2	$\frac{13}{48}$	0	$\frac{7}{48}$
			2	$\frac{5}{12}$	3	$\frac{7}{24}$	4	$\frac{3}{16}$		—
1d					0	$\frac{151}{240}$	1	$\frac{203}{480}$		—
					2	$\frac{91}{240}$	3	$\frac{9}{32}$	2	$\frac{19}{96}$
					4	$\frac{21}{80}$	5	$\frac{33}{160}$		—
1f							0	$\frac{1241}{2240}$		—
							2	$\frac{789}{2240}$	3	$\frac{13}{64}$
							4	$\frac{561}{2240}$		—
							6	$\frac{429}{2240}$		—
2s									0	$\frac{131}{192}$

TABLE VI

EXACT EXPRESSIONS FOR THE SLATER INTEGRALS

$R^k(v1,v\bar{1};v'1',v'\bar{1}')$ DIVIDED BY $e^2\lambda\sqrt{\frac{2}{\pi}}$

	k	$1s_{1/2}$	k	$1p_{3/2}$	k	$1p_{1/2}$	k	$1d_{5/2}$	k	$2s_{1/2}$	k	$1d_{3/2}$
$1s_{1/2}$	0	$\frac{5}{6}$	1	$\frac{7\sqrt{15}}{60}$	1	$\frac{1}{2}$	2	$\frac{3\sqrt{21}}{56}$	0	$\frac{\sqrt{15}}{48}$	2	$\frac{\sqrt{15}}{12}$
$1p_{3/2}$			0	$\frac{27}{40}$			1	$\frac{121\sqrt{35}}{1680}$	0	$\frac{27}{256}$	1	$\frac{11}{24}$
$1p_{3/2}$			2	$\frac{3}{8}$	2	$\frac{\sqrt{15}}{12}$	3	$\frac{11\sqrt{35}}{240}$			3	$\frac{7}{24}$
$1p_{1/2}$					0	$\frac{5}{6}$	3	$\frac{\sqrt{21}}{24}$	1	$\frac{\sqrt{15}}{80}$	1	$\frac{7\sqrt{15}}{60}$
$1d_{5/2}$							0	$\frac{1963}{3360}$				
$1d_{5/2}$							2	$\frac{1183}{3360}$	2	$\frac{57\sqrt{35}}{2240}$	2	$\frac{13\sqrt{35}}{240}$
$1d_{5/2}$							4	$\frac{819}{3360}$			4	$\frac{3\sqrt{35}}{80}$
$2s_{1/2}$									0	$\frac{1183}{1920}$		
$1d_{3/2}$											0	$\frac{27}{40}$
$1d_{3/2}$											2	$\frac{3}{8}$

APPENDIX B

PROGRAM FOR CALCULATION OF COULOMB ENERGIES

This program, written in the FORTRAN IV language, will print out the relativistic and non-relativistic oscillator constants λ, and calculate simultaneously the relativistic and non-relativistic Coulomb energies for closed shell nuclei (IHA = 1) or nuclei with one particle outside a closed shell (IHA = 2). The data cards must give the quantum numbers v, l, $\bar{l}$, and the sign of κ for each set of protons with the same values of these numbers, the total number of protons in the nucleus, the total number of neutrons, as well as certain numbers necessary for calculating the oscillator constants and for the READ and WRITE statements. The two cards giving the variables RO and SUM must be changed to correspond to the nucleus for which the calculation is to be made. The program prints out the Coulomb energy divided by $e^2\lambda$, $e^2\lambda$, and the Slater integrals and reduced matrix elements used to get the results.

```
      0C0000000011111111112222222222333333333344444444445555555556666666667777777778
      1234567890123456789012345678901234567890123456789012345678901234567890123456789
CARD
0001  C      PROGRAM FOR CALCULATION OF COULOMB ENERGIES
0002         REAL LAMSQ,MOVERE,MOVREP
0003         DIMENSION IV(100),XJ(20),ILB(20),ISK(20),IL(20)
0004  C      CALCULATION OF OSCILLATOR CONSTANT LAMBDA SQUARED
0005         DIMENSION Z(2), NMAX(2), LMAX(2), AXA(20), AYB(20)
0006         READ(5,100)(Z(I),I=1,2)
0007    100  FORMAT(2F5.1)
0008  C      A CARD GIVING THE RATIONAL NUMBER 'SUM' MUST BE INSERTED
0009  C      'SUM' IS THE AVERAGE OF 2V+L+3/2 FOR ALL PARTICLES
0010  C      RO, THE RADIUS PARAMETER, MUST BE GIVEN
0011         RO= 1.28
0012         SUM= 54./( 26.)
0013         AAMSQ= (3.*RO*RO/5.)*((Z(1)+Z(2))**(2./3.))
0014         LAMSQ=SUM/AAMSQ
0015         WRITE(6,5)Z(1),Z(2),LAMSQ
0016       5 FORMAT(1X,//,1X,'COULOMB ENERGIES FOR THE ELEMENT WITH Z =',F5.1,'
0017        1, N =',F5.1,///,1X,'THE OSCILLATOR CONSTANT LAMBDA SQUARED IS',E14
0018        2.7,//,1X)
0019         XBB= LAMSQ** 0.5
0020         XBB=XBB*(4.803)*( 4.803)/( 16.021)
0021         WRITE(6,11)XBB
0022      11 FORMAT(1X,'SCALE =',E14.7,' MEV')
0023      12 XMP=( 1.0545)*( 2.997925)/(( 1.6021)*( 9.38256))
0024         READ(5,6) NAX
0025       6 FORMAT(I3)
0026         READ(5,7)(AXA(I),AYB(I),I=1,NAX)
0027       7 FORMAT(20(2F7.4))
0028  C      AXA(I) = # OF PARTICLES WITH ENERGY CHARACTERIZED BY AYB(I), WITH SIGN
0029  C      OF LB-L, DIVIDED BY A
0030         ADS=SUM
0031       8 CORR= 0.0
0032         SUM=ADS
0033         DO 9 I=1,NAX
0034         FAC= 4.*LAMSQ*XMP*XMP
0035         WXYZ= 1.+FAC*AYB(I)
0036         EX= 1./(WXYZ** 0.5)
0037       9 CORR=CORR+(AXA(I)*( 1.-EX)*( 0.50))
0038         SUM=SUM+CORR
0039         XCA=LAMSQ-SUM/AAMSQ
0040         XCA=ABS(XCA)
0041         LAMSQ=SUM/AAMSQ
0042         IF(XCA.GE. 1.E-04)GO TO 8
0043         WRITE(6,10)LAMSQ
0044      10 FORMAT(1X,/,1X,'THE RELATIVISTIC LAMBDA SQUARED IS',E14.7,//,1X)
0045         XBB= LAMSQ** 0.5
0046         XBB=XBB*(4.803)*( 4.803)/( 16.021)
0047         WRITE(6,13)XBB
0048      13 FORMAT(1X,'RELATIVISTIC SCALE =',E14.7,' MEV')
0049         FAC= 4.*LAMSQ*XMP*XMP
0050  C      BEGIN MAIN PART OF COULOMB ENERGY CALCULATION
0051         READ(5,21)IHA,NJ
0052  C      IHA=1 FOR CLOSED SHELL NUCLEI, 2 FOR MIRROR NUCLEI
0053  C      NJ IS THE NUMBER OF SETS OF PARTICLES HAVING THE SAME J AND V
0054  C      (NOT COUNTING THE ODD PARTICLE, IF ANY)
```

80/80 LIST

```
      0000000001111111111222222222233333333334444444444555555555566666666677777777778
      1234567890123456789012345678901234567890123456789012345678901234567890123456789
CARD
0055      21 FORMAT(2I3)
0056         NHA=0
0057         EDE= 0.
0058         EXE= 0.
0059         ENDE= 0.
0060         EXNE= 0.
0061         READ(5,22)(IV(I),IL(I),ILB(I),ISK(I),I=1,NJ)
0062      22 FORMAT(40I2)
0063         READ(5,23)(XJ(I),I=1,NJ)
0064      23 FORMAT(16F5.1)
0065         IF(IHA.EQ.1)GO TO 24
0066         READ(5,22)IVC,ILC,ILBO,ISKO
0067         READ(5,23)XJO
0068      24 KK=1
0069         JK=1
0070      25 VI=IV(KK)
0071         VJ=IV(JK)
0072         LI=IL(KK)
0073         LJ=IL(JK)
0074         PAIRS=1.
0075         IF(KK.EQ.JK)GO TO 26
0076         PAIRS=2.
0077      26 XJA=XJ(KK)
0078         XJB=XJ(JK)
0079         WXYZ= 1.+FAC*(VI+XJA+1.)
0080         MOVERE= 1./(WXYZ** 0.5)
0081         WXYZ= 1.+FAC*(VJ+XJB+1.)
0082         MOVREP= 1./(WXYZ** 0.5)
0083         WRITE(6,27)MOVERE,MOVREP
0084      27 FORMAT(1X,'M/ E =',E14.7,//,1X,'M/EP =',E14.7)
0085  C      CALCULATION OF DIRECT ENERGIES
0086         IM= 2*IV(KK)+1
0087         IN= 2*IV(JK)
0088         CALL F(VI,VJ,LI,LJ,IM,IN,FK)
0089         WRITE(6,28)IV(KK),IV(JK),LI,LJ,FK
0090      28 FORMAT(1X,'F0(',4I3,') =',E14.7)
0091         ENDE=ENDE+FK*(XJA+0.5)*( 2.*XJB+1.)*PAIRS
0092         FK= 0.25*( 1.+MOVERE)*( 1.+MOVREP)*FK
0093         FK=FK*(XJA+0.5)*(2.*XJB+1.)*PAIRS
0094         EDE=EDE+FK
0095         LJ=ILB(JK)
0096         CALL F(VI,VJ,LI,LJ,IM,IN,FK)
0097         WRITE(6,28)IV(KK),IV(JK),LI,LJ,FK
0098         FA=FK
0099         FK= 0.25*(1.+MOVERE)*(1.-MOVREP)*FK
0100         FK=FK*(XJA+0.5)*(2.*XJB+1.)*PAIRS
0101         EDE=EDE+FK
0102         LI=ILB(KK)
0103         LJ=IL(JK)
0104         CALL F(VI,VJ,LI,LJ,IM,IN,FA)
0105         WRITE(6,28)IV(KK),IV(JK),LI,LJ,FA
0106         FK= 0.25*(1.-MOVERE)*(1.+MOVREP)*FA
0107         FK=FK*(XJA+0.5)*( 2.*XJB+1.)*PAIRS
0108         EDE=EDE+FK
```

```
CARD
0109        LI=ILB(KK)
0110        LJ=ILB(JK)
0111        CALL F(VI,VJ,LI,LJ,IM,IN,FK)
0112        WRITE(6,28)IV(KK),IV(JK),LI,LJ,FK
0113        FK= 0.25*(1.-MOVERE)*(1.-MOVREP)*FK
0114        FK=FK*(XJA+0.5)*(2.*XJB+1.)*PAIRS
0115        EDE=EDE+FK
0116        WRITE(6,29)XJA,XJB,ENDE,EDE
0117     29 FORMAT(1X,//,1X,'THE PARTIAL DIRECT ENERGY SUM UP TO JA =',F4.1,',
0118       1 JB =',F4.1,' IS',//,1X,E14.7,'(NONRELATIVISTIC)',//,1X,E14.7,'(RE
0119       2LATIVISTIC)')
0120  C     CALCULATION OF EXCHANGE ENERGIES
0121        XK=XJA-XJB
0122        XK=ABS(XK)
0123     30 LI=IL(KK)
0124        LJ=IL(JK)
0125        LK=LI
0126        LL=LJ
0127        XLA=LI
0128        XLB=LJ
0129        CALL REDMAT(XLA,XLB,XK,XJA,XJB
0130        IF(R.LT. 1.E-06)GO TO 35
0131        WRITE(6,31)LI,LJ,XK,XJA,XJB,R
0132     31 FORMAT(1X,//,1X,'C(',2I2,3F4.1,')  =',E14.7)
0133        IM=IV(KK)+IV(JK)
0134     32 CALL SL(VI,VJ,LI,LJ,LK,LL,IM,XK,SLK)
0135        WRITE(6,33)IV(KK),IV(JK),LI,LJ,LK,LL,SLK
0136     33 FORMAT(1X,//,1X,'G(',6I3,') =',E14.7)
0137        EXNE=EXNE+0.5*SLK*R*PAIRS
0138        SLK= 0.125*(1.+MOVERE)*(1.+MOVREP)*SLK*R
0139        EXE=EXE+SLK*PAIRS
0140        LK=ILB(KK)
0141        LL=ILB(JK)
0142        CALL SL(VI,VJ,LI,LJ,LK,LL,IM,XK,SLK)
0143        WRITE(6,33)IV(KK),IV(JK),LI,LJ,LK,LL,SLK
0144        SLK=0.25*(( 1.-MOVERE*MOVERE)*( 1.-MOVREP*MOVREP))** 0.5)*SLK*R
0145        XS=ISK(JK)*ISK(KK)
0146        EXE=EXE+SLK*XS*PAIRS
0147        LI=LK
0148        LJ=LL
0149        CALL SL(VI,VJ,LI,LJ,LK,LL,IM,XK,SLK)
0150        WRITE(6,33)IV(KK),IV(JK),LI,LJ,LK,LL,SLK
0151        SLK= 0.125*(1.-MOVERE)*( 1.-MOVREP)*SLK*R
0152        EXE=EXE+SLK*PAIRS
0153        WRITE(6,34)XJA,XJB,EXNE,EXE
0154     34 FORMAT(1X,//,1X,'THE PARTIAL EXCHANGE ENERGY SUM UP TO JA =',F4.1,
0155       1',JB =',F4.1,' IS',//,1X,E14.7,'(NONRELATIVISTIC)',//,1X,E14.7,'(R
0156       2ELATIVISTIC)')
0157     35 XK=XK+1.
0158        YK=XJA+XJB-XK
0159        IF(YK.LT.-1.E-06)GO TO 36
0160        GO TO 30
0161     36 IF(KK.GE.NJ.AND.JK.GE.NJ)GO TO 38
0162        IF(NHA.EQ.1)GO TO 37
```



```
CARD
0163        JK=JK+1
0164        IF(JK.LE.NJ)GO TO 25
0165     37 KK=KK+1
0166        IF(NHA.EQ.1)GO TO 25
0167        JK=KK
0168        GO TO 25
0169     38 IF(NHA.EQ.1)CALL EXIT
0170        NHA=NHA+1
0171        IF(NHA.EQ.2)GO TO 39
0172        WRITE(6,41)
0173        JK=JK+1
0174        IV(JK)=IVO
0175        IL(JK)=ILO
0176        ILB(JK)=ILBO
0177        ISK(JK)=ISKO
0178        XJ(JK)=XJO
0179        A=ENDE
0180        B=EDE
0181        C=EXNE
0182        D=EXE
0183        KK=1
0184        GO TO 25
0185     39 ENDE=(ENDE-A)/( 2.*XJO+1.)+A
0186        EDE=(EDE-B)/(2.*XJO+1.)+B
0187        EXNE=(EXNE-C)/( 2.*XJO+1.)+C
0188        EXE=(EXE-D)/(2.*XJO+1.)+D
0189        WRITE(6,40)ENDE,EXNE,EDE,EXE
0190     40 FORMAT(1X,//,1X,'THE FINAL COULOMB ENERGIES ARE',//,1X,E14.7,'(DIR
0191       1ECT NONRELATIVISTIC)',//,1X,E14.7,'(EXCHANGE NONRELATIVISTIC)',//,
0192       21X,E14.7,'(DIRECT RELATIVISTIC)',//,1X,E14.7,'(EXCHANGE RELATIVIST
0193       3IC)')
0194     41 FORMAT(1X,//,1X,'XXXXXXXXXX BEGIN CALCULATION FOR THE OCD PROTON')
0195        CALL EXIT
0196        END
0197  C
0198  C
0199        SUBROUTINE EHGF(XLA,XLB,XLC,XLD,XM,XN,XK,EGF)
0200  C     HYPERGEOMETRIC FUNCTION FOR THE EXCHANGE INTEGRALS
0201        DIMENSION A(100)
0202        EGF=1.
0203        I=1
0204        J=10
0205        X=(XLA+XLB+XLC+XLD)/(+2.0)+XN+XM+ 2.5
0206        XY=(XLA+XLB+2.*XN+XK+5.)/(+2.0)
0207        AXQW=X-XY
0208        AXQW=ABS(AXQW)
0209        IF(AXQW.LT. 1.E-06)GO TO 45
0210     41 DO 42 IN=I,J
0211        XIN=IN
0212        A(IN)=(X+XIN-1.)/(XY+XIN-1.)
0213        IF(IN.EQ.1)GO TO 42
0214        A(IN)=A(IN)*A(IN-1)
0215     42 CONTINUE
0216        AX=A(J)*( 0.5**J)
```

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80/80 LIST

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     12345678901234567890123456789012345678901234567890123456789012345678901234567890
CARD
0217       IF(AX.LT. 5.E-08)GO TO 43
0218       I=I+10
0219       J=J+10
0220       GO TO 41
0221    43 DO 44 JN=1,J
0222    44 EGF=EGF+A(JN)*( 0.5**JN)
0223       RETURN
0224    45 EGF= 2.
0225       RETURN
0226       END
0227  C
0228  C
0229       SUBROUTINE F(VI,VJ,LI,LJ,IM,IN,FK)
0230  C    THIS SUBROUTINE ASSEMBLES THE DIRECT INTEGRALS
0231       ZI=LI
0232       ZJ=LJ
0233       M=0
0234       N=0
0235       FK=0.
0236    10 XM=M
0237       XN=N
0238       XNC=XM+XN
0239       ARG=ZI+ZJ+2.5+XNC
0240       Y=GAMMA(ARG)
0241       Y=Y/(+2.**ARG)
0242       CALL AF(VI,VI,LI,LI,M,A)
0243       Y=Y*A
0244       CALL AF(VJ,VJ,LJ,LJ,N,B)
0245       Y=Y*B
0246       CALL DHGF(ZI,ZJ,XM,XN,LI,M,HGA)
0247       FAK=HGA/(ZJ+XN+1.5)
0248       CALL DHGF(ZJ,ZI,XN,XM,LJ,N,HGB)
0249  C    THE ARGUMENTS ARE STAGGERRED ON PURPOSE
0250       FAK=FAK+HGB/(ZI+XM+1.5)
0251       Y=FAK*Y
0252       M=M+1
0253       FK=FK+Y
0254       IF(N.EQ.IN.AND.M.EQ.IM)GO TO 11
0255       IF(M.NE.IM)GO TO 10
0256       N=N+1
0257       M=0
0258       GO TO 10
0259    11 FK=FK*(+0.25)
0260       ARGA=VI+ZI+1.5
0261       ARGB=VJ+ZJ+1.5
0262       ARGC=ZI+1.5
0263       ARGD=ZJ+ 1.5
0264       ARGVI=VI+1.
0265       ARGVJ=VJ+1.
0266       AA=GAMMA(ARGA)
0267       AB=GAMMA(ARGB)
0268       AC=GAMMA(ARGC)
0269       AD=GAMMA(ARGD)
0270       AVI=GAMMA(ARGVI)

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     12345678901234567890123456789012345678901234567890123456789012345678901234567890
CARD
0271       AVJ=GAMMA(ARGVJ)
0272       XNORM= 4.*AA*AB/(AVI*AVJ*AC*AC*AD*AD)
0273       FK=FK*XNORM
0274       RETURN
0275       END
0276  C
0277  C
0278       SUBROUTINE SL(VI,VJ,LI,LJ,LK,LL,IM,XK,SLK)
0279  C    THIS SUBROUTINE ASSEMBLES THE SLATER INTEGRALS FOR THE EXCHANGE ENERGY
0280       XLA=LI
0281       XLB=LJ
0282       XLC=LK
0283       XLD=LL
0284       M=0
0285       N=0
0286       SLK=0.
0287    14 XM=M
0288       XN=N
0289       XNC=XM+XN
0290       ARG=(XLA+XLB+XLC+XLD)/(+2.0)+XNC+2.5
0291       Y=GAMMA(ARG)
0292       Y=Y/( 2.**ARG)
0293       CALL AF(VI,VJ,LI,LJ,N,A)
0294       Y=Y*A
0295       CALL AF(VI,VJ,LK,LL,M,B)
0296       Y=Y*B
0297       CALL EHGF(XLA,XLB,XLC,XLD,XM,XN,XK,EGF)
0298       FAK=EGF/(XLA+XLB+2.*XN+XK+3.)
0299       CALL EHGF(XLC,XLD,XLA,XLB,XN,XM,XK,AGF)
0300  C    THE ARGUMENTS ARE STAGGERRED ON PURPOSE
0301       FAK=FAK+AGF/(XLC+XLD+2.*XM+XK+3.)
0302       Y=FAK*Y
0303       N=N+1
0304       IN=IM+1
0305       SLK=SLK+Y
0306       IF(N.EQ.IN.AND.M.EQ.IM)GO TO 15
0307       IF(N.NE.IN)GO TO 14
0308       M=M+1
0309       N=0
0310       GO TO 14
0311    15 SLK=SLK*( 0.5)
0312       XNORM= 1.
0313       IC=0
0314       XL=XLA
0315       V=VI
0316    16 IC=IC+1
0317       ARGA=V+XL+1.5
0318       ARGB=XL+1.5
0319       ARGV=V+1
0320       AA=GAMMA(ARGA)
0321       AB=GAMMA(ARGB)
0322       AV=GAMMA(ARGV)
0323       XZ=( 2.*AA/(AV*AB*AB))
0324       XZ=XZ** 0.5
```

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      00000000011111111112222222222333333333344444444455555555556666666667777777778
      12345678901234567890123456789012345678901234567890123456789012345678901234567890
CARD
0325        XNORM=XNORM*XZ
0326        XL=XLC
0327        GO TO (16,17,18,19),IC
0328     17 XL=XLB
0329        V=VJ
0330        GO TO 16
0331     18 XL=XLD
0332        GO TO 16
0333     19 SLK=SLK*XNORM
0334        RETURN
0335        END
0336  C
0337  C
0338        SUBROUTINE OHGF(XLA,XLB,XM,XN,LB,M,HGF)
0339        DIMENSION A(100)
0340  C     HYPERGEOMETRIC FUNCTION FOR THE DIRECT INTEGRALS
0341        HGF=1.
0342        I=LB+M
0343        IF(I.EQ.0)GO TO 35
0344        DO 32 J=1,I
0345        XJ=J
0346        A(J)= (-1.0)*(-(XLA+XM)+XJ-1.)/(XLB+XN+2.5+XJ-1.)
0347        IF(J.EQ.1)GO TO 32
0348        A(J)=A(J-1)*A(J)
0349     32 CONTINUE
0350        DO 34 J=1,I
0351     34 HGF=HGF+A(J)
0352     35 HGF=HGF*2.
0353        RETURN
0354        END
0355  C
0356  C
0357        SUBROUTINE AF(VI,VJ,LI,LJ,NC,AFG)
0358        DIMENSION A(50),B(50)
0359  C     BAILEY COEFFICIENTS FOR THE SUMS
0360        AFG=1.
0361        IF(NC.EQ.0)RETURN
0362        XLI=LI
0363        XLJ=LJ
0364        XNC=NC
0365        DO 52 J=1,NC
0366        XJ=J
0367        A(J)= (-VJ+XJ-1.)/(XJ*(XLJ+XJ+1.5-1.))
0368        B(J)= (-VI+XJ-1.)/(XJ*(XLI+XJ+1.5-1.))
0369  C     XJ GENERATES THE FACTORIAL
0370        IF(J.EQ.1)GO TO 52
0371        A(J)=A(J-1)*A(J)
0372        B(J)=B(J-1)*B(J)
0373     52 CONTINUE
0374        AFG=B(NC)+A(NC)
0375        IF(NC.EQ.1)RETURN
0376        NA=NC-1
0377        DO 53 IJ=1,NA
0378        IW=NC-IJ
```

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      12345678901234567890123456789012345678901234567890123456789012345678901234567890
CARD
0379     53 AFG=AFG+A(IJ)*B(IW)
0380        RETURN
0381        END
0382  C
0383  C
0384        SUBROUTINE REDMAT(XLA,XLB,XK,XJA,XJB,R)
0385  C     THIS SUBROUTINE FINDS THE SQUARE OF THE REDUCED MATRIX ELEMENT
0386  C     IT IS NECESSARY THAT THE TRIANGULAR CONDITIONS ARE SATISFIED OR ERRORS
0387  C     RESULT
0388        XN= 0.0
0389        S= 1.
0390     32 Y=XN-(XLA+XLB+XK)
0391        Y=ABS(Y)
0392        IF(Y.LT. 1.E-06)GO TO 33
0393        XN=XN+1.
0394        S=-S
0395        GO TO 32
0396     33 IF(S.GT. 0.)GO TO 34
0397  C     IF L+L'+K IS ODD  , THEN THE REDUCED MATRIX ELEMENT IS ZERO
0398  C     RETURN IS MADE TO STATEMENT 35 TO AVOID USELESS STEPS
0399        R= 0.0
0400        RETURN
0401     34 AA=XJA+XJB-XK+1.0
0402        AAA=GAMMA(AA)
0403        AB=XJA+XK-XJB+1.0
0404        ABB=GAMMA(AB)
0405        AC=XJB+XK-XJA+1.0
0406        ACC=GAMMA(AC)
0407        AD=XJA+XJB+XK+2.0
0408        ADD=GAMMA(AD)
0409        DELTSQ=(AAA*ABB*ACC)/ADD
0410        XN= 0.
0411        S=1.
0412     35 Y=XN-(XJA+XJB+XK)
0413        Y=ABS(Y)
0414        IF(Y.LT. 1.E-06)GO TO 36
0415        XN=XN+1.
0416        S=-S
0417        GO TO 35
0418     36 IF(S.GT. 0.)GO TO 37
0419        AD= 0.5*(XK+XJB+XJA+3.0)
0420        AC= 0.5*(XJB+XK-XJA+2.0)
0421        AB= 0.5*(XJA+XK-XJB+2.0)
0422        AA= 0.5*(XJA+XJB-XK+1.0)
0423        GO TO 38
0424     37 AD= 0.5*(XK+XJA+XJB+2.0)
0425        AC= 0.5*(XJB+XK-XJA+1.0)
0426        AB= 0.5*(XJA+XK-XJB+1.0)
0427        AA= 0.5*(XJA+XJB-XK+2.0)
0428     38 ADD=GAMMA(AD)
0429        ACC=GAMMA(AC)
0430        ABB=GAMMA(AB)
0431        AAA=GAMMA(AA)
0432        FO=ADD/(AAA*ABB*ACC)
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      C0000000011111111112222222222333333333344444444455555555556666666667777777778
      1234567890123456789012345678901234567890123456789012345678901234567890123456789
CARD
0433          FQ=FQ*FQ
0434          R= 4.0*DELTSQ*FQ
0435          RETURN
0436          END
0437  C
0438  $ENTRY
0439    7.0  6.0
0440    2
0441   0.2308 1.5000 0.6154 2.5000
0442    2  2
0443   0 0 1-1 0 1 2-1
0444    0.5  1.5
0445   C 1 0 1
0446    0.5
0447  $IBSYS
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VITA

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