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Configurations

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Collective motion in the nuclear shell model

I. Classification schemes for states of mixed configurations

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To understand how collective motion can develop in the shell-model framework it is necessary to study configuration interaction. With this in mind, group-theoretical methods are used to investigate the possible classification schemes for a number of nucleons in mixed configurations. One particular coupling scheme, which is associated with the degeneracy of a harmonic oscillator potential and which, in a following paper, will be shown to have collective properties is described in detail. The wave functions in this scheme are seen to be very similar to those resulting from an actual shell-model calculation with configurational mixing.

1. Introduction

Because of the complexity of the many-body problem and the lack of knowledge of the fundamental inter-nucleon interaction, simple models of the nucleus have been constructed in an attempt to correlate the experimental data and perhaps lead the way to a more rigorous theory. The most successful of these have been the rotational model and the individual particle (or shell) model. Each of these models has a number of versions and in their simplest extreme versions the two models are quite distinct. One uses the picture of a rotating body and the other that of a single particle moving in a spherically symmetric potential well. However, these simple versions enjoy only a limited success which has led to the development of more complicated versions of the models. In the rotational model the particle structure of the nucleus has been taken into account by Nilsson (1955) who puts nucleons into a deformed potential well which is then assumed to rotate adiabatically. In the shell model the interaction between all pairs of particles has been included, and where different configurations lie close together their mixing has been taken into account as, for example, in ¹⁹F (Elliott & Flowers 1955). It is no longer clear that in these generalized versions the two models are distinct. For example, if we allow all possible configuration mixing in the shell model we have a complete set of states which though infinite is in principle capable of describing a rotational model. The important problem is to see if collective properties, and in particular rotational properties, can emerge from the usual type of shell model calculation with only that very limited amount of configuration mixing from nearby configurations which has been found necessary (in ¹⁹F for example) to explain the experimental data. This problem is studied in the present series of papers and we shall see that rotational properties do emerge from a particularly simple type of configuration mixing.

Empirically it is clear that the two models are related in some way because they may both be used, with equally good results, in accounting for the properties of certain light nuclei. The intermediate coupling version of the shell model has been very successful in the (1p) shell (Kurath 1956) for nuclei with 4 < A < 16 and also

beyond ¹⁶O for such nuclei as ¹⁹F. In the latter work, however, the nucleons outside the closed ¹⁶O shell may lie in either the (1d) or (2s) orbits which are degenerate in energy for the oscillator potential. If the oscillator potential is a reasonable approximation in these nuclei, as is believed, there will therefore be strong mixing between such configurations as $d^n, d^{n-1}s, \ldots, d^{n-4}s^4$. In the work on ¹⁹F this was found to be the case. Beyond ²⁰Ne the number of possible states from all such configurations becomes very large, making similar intermediate coupling calculations prohibitively laborious. In this same region of mass number the nucleus ²⁴Mg has been found to have a nearly rotational spectrum. Furthermore, the version of the rotational model developed by Nilsson (1955) has been remarkably successful in explaining the more detailed experimental data available for the neighbouring nuclei ²⁵Mg and ²⁵Al (Litherland, Paul, Bartholomew & Gove 1956). For example there are about twelve levels known, and although they do not all belong to the same rotational band they may be fitted to a series of bands with different values of K. (In the rotational model, K is the projection of angular momentum on the symmetry axis of the body or potential well. For each intrinsic state with a given value of K, which is a good quantum number, there is a spectrum of levels with J = K, K+1, K+2, etc., except for K = 0 when J must be even or odd according to the parity of the state.) Nilsson's model predicts correctly the values of K which should occur, and these assignments are corroborated by the observed decay data which confirm selection rules in K also predicted by Nilsson. This model has also been applied with success to ¹⁹F (Paul 1957), and even to the 1p-shell nuclei where the shell model has had its major successes.

The situation is therefore a challenging one. It suggests that there is some connexion between the shell model as applied to these light nuclei on the one hand, and Nilsson's version of the rotational model on the other. In particular, it implies that the shell model wave functions for 19F, which are the result of configuration mixing, bear some close relation to rotational wave functions. If this is indeed the case then there should be some underlying ideal coupling scheme which exhibits the rotational properties ab initio. Just as the concept of seniority (Racah 1943; Flowers 1952) brings out the single-particle features for states of particles in a pure configuration, we must now look for some quantum numbers which bring out the rotational features for states of particles in mixed configurations. In particular, we shall be interested in the mixed configurations of degenerate oscillator orbits because, at least for the light nuclei, this is likely to be the most important mixing. A search for possible quantum numbers is necessarily a search for the possible classification schemes, or in other words, a study of the possible transformation properties of the wave functions. The angular momentum L may be looked upon as describing the transformation properties of the wave function under three-dimensional rotations in co-ordinate space. We must study more general groups of transformation than this. Fortunately, Racah has developed very powerful methods for such a study, and although he has only applied them to pure configurations they may also be used for mixed configurations.

For the sake of simplicity we shall restrict our attention to the L-S coupling extreme. If we can understand the connexion between this extreme and the rotational model it should be possible to include the spin-orbit force, which tends to

destroy L-S coupling, at a later stage. In this extreme it has been known for a long time (Feenberg & Phillips 1937) that, for any spin-independent force, the levels of a given partition [f] of the p^n configuration have energies proportional to L(L+1). This situation actually occurs in ${}^8\mathrm{Be}$ (Kurath 1956) and is obscured in other p-shell nuclei only by the spin-orbit force. This is exactly the feature that we are looking for, namely a rotational spectrum. In the d^n configuration this rotational spectrum does not appear; but since we know that the (1d) and (2s) shells are mixed it is possible that such a spectrum may nevertheless emerge for some particular type of mixing. The empirical evidence mentioned earlier suggests that it does. It is significant here that the (1p) shell is the only non-degenerate one in the oscillator well, apart from the trivial (1s) shell. In the only case where there can be no mixing of degenerate oscillator levels the rotational structure appears.

This paper first describes a general method for studying the classification schemes of mixed configurations and then concentrates on a particular scheme which is applicable to the degenerate configurations of an oscillator potential. This coupling scheme, associated with the group U_3 of three-dimensional unitary transformations, is a generalization of that used in the pure p-shell. There it coincides with the classification of the states by the permutation symmetry of their orbital wave functions denoted by the partition [f]. The U_3 coupling scheme groups together states whose L-values are just those of rotational bands cut off at some upper value of L. A comparison is made between the wave functions from certain mixed-configuration shell-model calculations and those of the U_3 coupling scheme, the result being a great similarity between the functions from the two sources. This means that the classification is of physical significance. It is important to demonstrate this at least in a number of particular examples, for hitherto the classification has been considered merely as a mathematical device.

A following paper shows very clearly that the U_3 wave functions have rotational properties by expressing them as Hill–Wheeler integrals (Hill & Wheeler 1953) over certain intrinsic states. The band structure mentioned above is now explained, because all states of a given band are shown to involve the same intrinsic state in this integral. Using this integral formulation it is possible to derive explicit formulae for the matrix elements of the electric quadrupole operator which in the limit of many particles tend towards the formulae of the rotational model. Even for a few particles this limit is closely approximated.

In a further paper the integral form is used to derive fractional parentage coefficients in a simple way, and the problem of the energy matrix is also considered. Although the U_3 classification is a generalization of that for the p-shell, it is no longer true that any spin-independent force gives a rotational spectrum as in the p-shell. However, it does seem that a nearly rotational spectrum is produced with the usual kind of two body force used in shell model calculations.

2. The search for coupling schemes

Racah (1949, 1951) has developed group-theoretical methods for studying the classification of states of configuration l^k . These methods have been applied by Jahn (1950) to the d^k configurations in L-S coupling and by Flowers (1952) to the

configurations j^k in the j-j coupling approximation. In this section we generalize the method to a mixed configuration, and for simplicity we consider the mixing of just two different orbital shells l_a and l_b . We want to investigate the possible ways of classifying the states of k particles which may be in either of these orbits. One way would of course be to make each state belong to some definite configuration $l_a^r l_b^{k-r}$; but there will be other schemes in which the states are linear combinations of functions belonging to different configurations, i.e. to different values of r.

The wave functions $\phi(lm)$ of a single particle in either of these orbits span a vector space of s dimensions, where $s=(2l_a+1)+(2l_b+1)$. Consider therefore the most general group of transformations in this space which preserves the orthonormality of the functions, namely the group U_s of unitary transformations in this space. The infinitesimal operators of this group, which are s^2 in number, may be denoted by $E_{mm'}^{ll'}$, where $E_{mm'}^{ll'}\phi(l''m'')=\delta(l'l'')\,\delta(m'm'')\,\phi(lm). \tag{1}$

We may of course define these operators in a variety of ways by taking linear combinations of them. Since it is always convenient to know the transformation properties of operators under three-dimensional rotations, in other words to deal with tensor operators in the sense used by Racah (1942), we define an equivalent set of operators $u_0^{\alpha}(ll')$ by the relations

 $u_{q}^{(l)}(ll') = \frac{1}{\sqrt{(2l+1)}} \sum_{m,m'} (l'tm'q \mid l'tlm) E_{mm'}^{ll'}.$ $t = (l+l'), (l+l'-1) \dots \mid l-l' \mid,$ $q = t, (t-1), \dots, -t,$ (2)

Here

and $(l'tm'q \mid l'tlm)$ is a Wigner coefficient. The operators $u_q^{(l)}(ll')$ are now irreducible tensor operators in the sense used by Racah (1942) and have simple known properties under rotation of the co-ordinate system, viz. they transform like the spherical harmonics $Y_q^{(l)}$. Consequently they are completely defined by their amplitude matrices $(l''' \parallel \mathbf{u}^{(l)}(ll') \parallel l'') = \delta(ll''') \delta(l'l'') \tag{3}$

from which any matrix element may be derived in the usual way (Racah 1942),

$$(l'''m''' \mid u_q^{(l)}(ll') \mid l''m'') = (2l+1)^{-\frac{1}{2}}(l''tm''q \mid l''tl'''m''') \,\delta(ll''') \,\delta(l'l'').$$

In the theory of continuous groups a set of infinitesimal operators describes a group if their commutators are also operators of the set. From the definitions (1) and (2) the commutators of the operators $u_q^{(l)}(ll')$ are given by the equations*

$$\begin{split} [u_q^{(t)}(ll'),\, u_p^{(s)}(kk')] &= \sum\limits_{r,\,v} (2r+1)^{\frac{1}{2}}(tsqp \mid tsrv) \\ &\times \{(-1)^{t+s-r}\delta(l'k) \; W(tslk'\,;rl') \, u_v^{(r)}(lk') - \delta(lk') \; W(tsl'k\,;rk') \, u_v^{(r)}(kl')\}, \quad (4) \end{split}$$

where W denotes the Racah function which arises in this case from a sum over three Wigner coefficients. Equation (4) demonstrates that the operators $u_q^{(l)}(ll')$ do in fact describe a group. If we now form many-body operators

$$U_q^{(t)}(ll') = \sum_{i=1}^k u_q^{(t)}(ll'; i), \tag{5}$$

^{*} In (4), the symbols s and k are not to be confused with those used earlier in this section for the number of single-particle functions and the number of particles, respectively.

where $u_q^{(l)}(ll';i)$ operates only on particle i, then it follows that the $U_q^{(l)}(ll')$ also satisfy (4). The operators $U_q^{(l)}$ describe a simultaneous transformation of all particles. This transformation therefore induces a transformation among the many-particle wave functions ψ of the k-particle system, and enables us to classify these functions according to the irreducible representations of the group U_s . Whereas the single particle function ϕ is a vector in the s-dimensional space, the k-particle functions ψ are tensors of rank k. This classification is identical with the supermultiplet classification of Wigner, the states being labelled by a partition [f] of k into s parts. The states which spread out the irreducible representation [f] of the symmetric group S_k of particle permutations also transform according to the irreducible representation [f] of the group U_s under simultaneous unitary transformations of all particles (see Weyl 1928, p. 281). To each partition there is then an associated set of spin and isotopic spin functions which, combined with the orbital functions ψ , which are not necessarily antisymmetric, form a totally antisymmetric function (cf. Jahn 1950).

If we can find a subset of the operators $U_{\sigma}^{(l)}(ll')$ whose commutators also belong to that subset, then the subset of operators describes a subgroup of the original group U_s . It then follows that the states ψ may be classified simultaneously according to irreducible representations of both the full group U_s and its subgroup. Such a process enables us to distinguish states belonging to the same irreducible representation of the group U_s . The orbital angular momentum operators L_q are always contained in the full set of operators $U_q^{(l)}(ll')$. Because these operators L_q are also the infinitesimal operators of the group R_3 of rotations in orbital space it follows that the group R_3 is a subgroup of U_s . Thus the quantum number L, which labels the irreducible representations of R_3 may be used in addition to [f] to classify the states. So far we have used group-theoretical language only to describe the supermultiplet classification for the mixed configuration in L-S coupling. However, we can now go further. For a given l_a and l_b we can search for a subset of the operators $U_a^{(t)}(ll')$ which satisfies the group conditions and which contains the operators L_q of R_3 . If such a set can be found it will describe a subgroup G of U_s which contains R_3 as a subgroup.

Consequently we may use the irreducible representations of G in addition to those of U_s and R_3 to classify the k-particle states ψ . It is certainly necessary to introduce some label in addition to [f] and L because for more than a very few particles there will be more than one state having the same values for [f] and for L. Racah (1949) and Jahn (1950) used this approach to introduce the seniority quantum number for a pure l^k configuration, and Flowers (1952) used it for a pure j^k configuration in the j-j coupling approximation. The groups involved were R_{2l+1} and Sp_{2j+1} respectively. Here we shall apply the method to mixed configurations in L-S coupling.

For any values of l_a and l_b it may be shown that the set of operators

$$u_q^{(t)}(l_a l_b) + u_q^{(t)}(l_b l_a),$$

with $u_a^{(t)}(l_a l_a)$ and $u_a^{(t)}(l_b l_b)$ for odd values of t,

describe the group R_s of orthogonal transformations in the s-dimensional space. This allows the formal introduction of the concept of seniority for mixed configurations, but no physical significance has yet been found for such a classification. Further discussion of the group R_s and its associated coupling scheme is therefore deferred until the appendix, where the particular case of $l_a = 0$, $l_b = 2$ is described. In the rest of this paper we shall be concerned with a subgroup U_3 of U_s which may be used when the mixing orbits l are those of a degenerate oscillator level.

3. The degenerate oscillator configurations

The average central potential of the shell model is believed to resemble a harmonic oscillator potential for light nuclei, with single particle energy levels

$$1s; 1p; 2s, 1d; 2p, 1f; 3s, 2d, 1g; ...;$$
 etc.

The levels between successive semi-colons above are degenerate in energy and therefore the mixing of these orbital shells is expected to be physically important. In particular, the (2s) and (1d) shells will be expected to mix strongly in nuclei having 16 < A < 40, while the mixing between the (2p) and (1f) shells will be expected to be important in determining the spectra of nuclei with 40 < A < 80. The general methods outlined above show that the group U_3 of three-dimensional unitary transformations may be used in both these cases. In fact this group may be used in classifying the states of particles in any degenerate oscillator configuration. We use the term degenerate oscillator configuration to include all configurations obtained by putting a given number of particles into any of the orbital levels which are degenerate.

This property of the group U_3 may be seen in the following direct way as a result of the symmetry of the oscillator Hamiltonian

$$H_0 = r^2 + b^4 p^2$$
.

Here b is the scale parameter of the wave functions, the first few of which we give below for reference:

$$\begin{aligned} u_{1s}(r) &= (2/\pi^{\frac{1}{4}}) \exp\left(-r^2/2b^2\right), \\ u_{1p}(r) &= (2\sqrt{2}/\pi^{\frac{1}{4}}\sqrt{3}) \left(r/b\right) \exp\left(-r^2/2b^2\right), \\ u_{1d}(r) &= (4/\pi^{\frac{1}{4}}\sqrt{15}) \left(r^2/b^2\right) \exp\left(-r^2/2b^2\right), \\ u_{2s}(r) &= (\sqrt{2}/\pi^{\frac{1}{4}}\sqrt{3}) \left\{2(r^2/b^2) - 3\right\} \exp\left(-r^2/2b^2\right). \end{aligned}$$
 (6)

The oscillator Hamiltonian H_0 is invariant, not only with respect to rotations but also with respect to the more general group U_3 described by the nine operators

$$H_{0} = r^{2} + b^{4}p^{2},$$

$$L_{q} = (\mathbf{r} \times \mathbf{p})_{q},$$

$$Q_{q} = (4\pi/5)^{\frac{1}{2}} \{ r^{2} Y_{q}^{(2)}(\theta_{r}, \phi_{r}) + b^{4}p^{2} Y_{q}^{(2)}(\theta_{p}, \phi_{p}) \} / b^{2}.$$
(7)

Here the L_q are the three rotation operators and the Q_q the five components of a second degree tensor operator. The arguments of the spherical harmonics above are the polar angles of the vectors \mathbf{r} and \mathbf{p} respectively. In particular

$$Q_0 = \{(2z^2 - x^2 - y^2) + b^4(2p_z^2 - p_x^2 - p_y^2)\}/2b^2.$$

The numerical constant in Q_q is for later convenience, and we have made Q_q dimensionless. The invariance of H_0 with respect to the group U_3 is equivalent to saying that it commutes with the operators (7) of the group. This invariance was pointed out by Jauch & Hill (1940) and is responsible for the well-known degeneracy. The degenerate levels belong to the same irreducible representation of U_3 . In other words, the group operators transform between the degenerate orbital states only. This may be seen immediately from the fact that the operators (7) are the nine products of the three creation operators $(\mathbf{r}-\mathrm{i}b^2\mathbf{p})$ and the three destruction operators $(\mathbf{r}+\mathrm{i}b^2\mathbf{p})$ of the oscillator quanta. Such product operators must clearly leave the energy unchanged. It is now obvious that this group U_3 is of the kind for which we are searching. It contains R_3 as a subgroup so that a definite value for the total orbital angular momentum L may be given to each state and if the l_a, l_b , etc., are the l-values occurring in a degenerate oscillator level then it is contained in U_s as a subgroup. When there are more than two l-values s is of course generalized to

$$s = (2l_a + 1) + (2l_b + 1) + \dots$$

It may be verified directly from the commutation relations of the operators (7) that they describe the group U_3 . We find

$$\begin{split} [L_{q},L_{q'}] &= -\sqrt{2}(11qq' \mid 111q+q') \, L_{q+q'}, \\ [Q_{q},L_{q'}] &= -\sqrt{6}(21qq' \mid 212q+q') \, Q_{q+q'}, \\ [Q_{q},Q_{q'}] &= 3\sqrt{10}(22qq' \mid 221q+q') \, L_{q+q'}. \end{split}$$
 (8)

In the oscillator shell with quantum number N, corresponding to an energy of $(N+\frac{3}{2})$, the expression of these operators in terms of the $u_q^{(l)}(ll')$ of the last section is given by the relations

$$L_{q} = \sum_{l} \{l(l+1) (2l+1)\}^{\frac{1}{2}} u_{q}^{(1)}(ll),$$

$$Q_{q} = \sum_{l} \left[-(2N+3) \left\{ \frac{l(l+1) (2l+1)}{(2l-1) (2l+3)} \right\}^{\frac{1}{2}} u_{q}^{(2)}(ll) + \left\{ \frac{6(l+1) (l+2) (N-l) (N+l+3)}{(2l+3)} \right\}^{\frac{1}{2}} \times \left\{ u_{q}^{(2)}(l,l+2) + u_{q}^{(2)}(l+2,l) \right\} \right].$$
(9)

the summation extending over the degenerate orbital shells with

$$l = N, N-2, N-4, ..., 1$$
 or 0.

Whereas the L_q generate infinitesimal rotations of the co-ordinate system the Q_q are related to the operators of infinitesimal quadrupole distortions.

4. The classification according to the group U_3 .

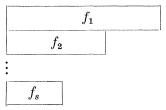
In an oscillator shell, the existence, as a subgroup of U_s , of the group U_3 which contains the group R_3 of co-ordinate rotations as a subgroup, means that the states ψ of k particles in such a shell may be classified simultaneously according to representation of the three groups. As in §2 we must then construct the many-particle operators $L_q = \sum_{i=1}^k L_q(i),$

 $Q_q = \sum_{i=1}^k Q_q(i),$

where of course L is the total orbital angular momentum. (Although we used the symbols L_q and Q_q for single particle operators in §3 and many particle operators here, the distinction will be obvious from the context.)

The irreducible representations of the group U_s are labelled by a set of s numbers $f_1, f_2, ..., f_s$ such that $f_1 \ge f_2 \ge ... \ge f_s$,

and where the f_i are positive integers or zero. The set may be looked upon as a partition of the sum $\sum_{i=1}^{s} f_i$ and illustrated by a tableau having f_i blocks in the *i*th row. We



have used the abbreviated notation [f] for this set of numbers. In physical problems we want to ignore transformations which are simply an overall change of phase and this means dealing with the unimodular unitary group SU_s obtained by removing the unit infinitesimal operator. Under this restriction the representations do not reduce further, but those corresponding to tableaux differing only in a number of complete columns become equivalent (Weyl 1928, p. 389). Thus for the unimodular unitary group SU_3 the irreducible representations may be labelled by only two numbers f_1 and f_2 . For convenience we use the equivalent pair of numbers $\lambda = f_1 - f_2$ and $\mu = f_2$ to label the representations of SU_3 by the symbol $(\lambda \mu)$.

As explained in § 2 the classification according to irreducible representations of the full group SU_s is identical with the supermultiplet classification. Both use the partition [f] of the number of particles as a label. When we restrict the group of transformations from SU_s to SU_3 the representations [f] are still representations of the subgroup SU_3 but are no longer irreducible. In general they may be reduced to a sum over certain irreducible representations $(\lambda\mu)$ of SU_3 . In the same way on further restriction from SU_3 to R_3 the representations $(\lambda\mu)$ will reduce further into irreducible representations of R_3 , labelled by the total orbital angular momentum L. The problem of classifying the states is therefore the problem of determining which representations $(\lambda\mu)$ occur in a given representation [f] and which values of L occur in a given $(\lambda\mu)$. This is a well-defined mathematical problem which will be discussed in § 5.

Table 1 contains the complete classification of states in the N=2 oscillator shell for $k \le 4$. For k > 4 only those states are given which belong to the two lowest partitions in the Wigner approximation, i.e. those having the higher orbital symmetries which are found to occur lowest in energy when the interactions are mainly composed of Wigner and Majorana forces. Table 2 contains the complete set of states in the N=3 shell for $k \le 4$ only. It is a straightforward matter to extend the range of these tables as required. In the tables we list the values of $(\lambda \mu)$ which occur in each partition [f]. The values of L which occur in each representation $(\lambda \mu)$ follow from a simple explicit rule (14) and so are not listed in the tables. A few examples are

Table 1. The classification of the orbital states of the combined $1d$ and $2s$ shells using the group U_3	(For convenience, the table is presented in three parts, according to whether the number $k+2$, $k+1$, or k is divisible by 3. We tabulate the number of times that each representation $(\lambda \mu)$ appears in the reduction of a given representation $[f]$.)

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(75)		(84		(2,0)	
(10, 2		(11, 1	· · · · · · · · · · · · · · ·	$(\lambda\mu)(12,0)$ (93) (66) (39)	
$(\lambda \mu)$ $(10, 2)$ (75) (48) $(11, 0)$	[1] [81] [22] [22] [111] [43] [42] [42]	$(\lambda \mu)$ (11, 1) (84) (57) (2, 10	[7] [11] [41] [32] [44] [44] [42]]	ης) [£]	[3] [21] [42] [441] [444] [444]
' ਣੋ '	[1] [2] [22] [22] [21] [1111] [43] [442] [442]	₹,		Z.	$\begin{bmatrix} 3 \\ 6 \\ 9 \end{bmatrix}$
7	1 4 7 10	7	11 8 21 13 8		7

given in § 5. It is here that we first see a rotational structure appearing, the L-values from (14) being just those of a series of rotational bands cut off at some upper limit. To each orbital state L of a partition [f] there corresponds a supermultiplet of spin and isotopic spin values, but these are of course independent of the orbital wave functions and may be taken from the work of Jahn (1950), for example. The effectiveness of the classification in distinguishing the states is clear from table 1. For $k \le 4$ the same representation $(\lambda \mu)$ never occurs more than once in a given partition [f], and for greater values of k the representations $(\lambda \mu)$ with highest values of $k + \mu$ are always unique. This is very satisfactory because we shall see in a later paper that such representations correspond to states which lie lowest in energy when a reasonable inter-nucleon force is included. Within a representation $(\lambda \mu)$ it is clear from (14) that when min $\{\lambda, \mu\} \ge 2$ there will be more than one state with the same value for L. At this stage we have no systematic way of separating such states, although this may be done in any arbitrary way. However, in the following paper we shall find a very natural way of separating these states by means of a Hill-Wheeler integral.

The tables all refer to the first half of the shell, but the results for the second half follow simply by considering k holes instead of k particles and interchanging λ and μ in the partition obtained by writing $4-f_{s-i}$ for f_i .

Although we have discussed the U_3 classification in terms of oscillator wave functions, the same classification may be used whatever the form of the single particle radial wave functions. We may formally define the operators $u_q^{(b)}$ by (1) and (2) in terms of any radial wave function, although the *explicit* form of these operators given by (7) is only true for oscillator wave functions. For example, if we took the radial wave functions to be homogeneous polynomials, then the eight operators of SU_3 would be given by L_q as before and by $Q_q \propto (r \times q)_q^{(2)}$.

Table 2. The classification of the orbital states of the combined 1f and 2p shells using the group U_3

```
[f]
n
                                                            (\lambda \mu)
0
        [0]
                 (00)
1
        \lceil 1 \rceil
                 (30)
        [2]
                 (60)(22)
       [11]
                 (41)(03)
3
        [3]
                 (90) (52) (33) (30) (03)
       [21]
                 (71) (52) (33) (41) (14) (22) (11)
     [111]
                 (60) (33) (22) (00)
4
                 (12, 0) (82) (63) (44) (60) (33) (41) (06) (22) (00)
        [4]
       [31]
                 (10, 1) (82) (63)^2 (71) (44) (52)^2 (60) (25)^2 (32)^2 (41)^2 (14) (22)^2 (30) (03) (11)
       [22]
                 (82) (71) (44)^2 (52) (60) (33) (41) (06) (14) (22)^2 (11)
     [211]
                 (90) (63) (71) (44) (52)^2 (25) (33)^2 (41)^2 (14)^2 (22) (30)^2 (03) (11)
    [1111]
                 (52) (33) (06) (22) (30)
```

5. The restrictions from $SU_{\!\scriptscriptstyle S}$ to $SU_{\!\scriptscriptstyle 3}$ and from $SU_{\!\scriptscriptstyle 3}$ to $R_{\!\scriptscriptstyle 3}$

To determine which irreducible representations of a subgroup occur in an irreducible representation of the original group we must first know how a product representation reduces in each group. For the group R_3 there is the well-known Clebsch–Gordon relation (cf. Weyl 1928, p. 190).

$$D_L \! \times \! D_{L'} = D_{L\!+\!L'} \! + \! D_{L\!+\!L'\!-\!1} \! + \ldots + D_{|L\!-\!L'|},$$

which tells us which representations occur when the (2L+1)(2L'+1) — dimensional product representation is reduced. This is simply the rule for vector-coupling angular momenta. There is no such simple formula to describe the reduction of product representations in the unitary group. However, the reduction may be obtained quite simply in any particular case by using certain rules for combining the tableaux which describe the representations (Littlewood 1940; Jahn 1950). A simple example for the group SU_3 is

$$(\lambda \mu) \times (10) = (\lambda + 1, \mu) + (\lambda - 1, \mu + 1) + (\lambda, \mu - 1). \tag{11}$$

Such reductions as this may always be checked by comparing the total dimension of the representations on each side of the equation. For example in the rotation group R_3 the representation D_L is of (2L+1) dimensions and it is easily seen that the sum of these dimensions on the right-hand side of (10) is just (2L+1)(2L'+1). The same thing may be done for the unitary groups using the formula (Weyl 1928, p. 383),

dimension of $[f] = \prod_{1 \le i < j \le s} \left(\frac{f_i - f_j + j - i}{j - i} \right)$ (12)

for the dimension of the irreducible representations [f] of U_s or of SU_s .

The representations ($\lambda 0$) describe the unitary transformation properties of tensors of rank λ in the three-dimensional space. Thus, for example, (00) corresponds to a scalar and (10) to a vector. In the reduction from SU_3 to R_3 therefore, these two simple representations do not break up, but are given the labels D_0 and D_1 appropriate to the group R_3 . Hence in the language of the classification of states, the representation (00) contains a single S state, while (10) contains a single S state. From this starting-point, and using the formulae (10) and (11), it is now possible to determine which values of L occur in a given representation ($\lambda \mu$). Use is also made of the fact that the representations ($\lambda \mu$) and ($\mu \lambda$) contain the same L-values, although the actual states are not identical. Interchanging λ and μ corresponds to replacing particles by holes. An example illustrates the process.

From (11) we have, for $\lambda = 1$, $\mu = 0$, the reduction

$$(10) \times (10) = (20) + (01). \tag{13}$$

From equation (10), however, knowing that the representation (10) contains D_1 alone, it follows that the right-hand side of (13) must contain D_2 , D_1 and D_0 . Since (01) contains D_1 we have the result that (20) contains D_2 and D_0 . This result may be checked by comparing the dimension of the representation (20) with the sum of the dimensions of D_2 and D_0 . In this same way from the product (10) × (01) we find that (11) contains D_1 and D_2 and the process may be extended indefinitely. A general rule emerges from this procedure which may be expressed as follows.

The representations D_L which occur in the representation $(\lambda \mu)$ of SU_3 are given by

$$L = K, (K+1), (K+2), \dots (K + \max\{\lambda, \mu\}), \tag{14}$$

where the integer $K = \min \{\lambda, \mu\}, \min \{\lambda, \mu\} - 2, ..., 1 \text{ or } 0$, with the exception that if K = 0 $L = \max \{\lambda, \mu\}, \max \{\lambda, \mu\} - 2, ..., 1 \text{ or } 0.$

This result shows clearly that the values of L within a representation are just those of a series of rotational bands cut off at $L = K + \max\{\lambda, \mu\}$. For example if $\mu = 0$ and λ is even we have a single K = 0 rotational band with

$$L = 0, 2, 4, ..., \lambda,$$

while if $\mu = 1$ we obtain a K = 1 band with

$$L = 1, 2, 3, ..., (\lambda + 1).$$

The parameter K used in (14) would correspond to the projection of the angular momentum on the symmetry axis in the rotational model. In the following paper we shall show how the wave functions of this U_3 classification may be written as Hill–Wheeler integrals over intrinsic states. Then, the parameter K will arise naturally as such a quantum number of the intrinsic state. When $\min\{\lambda,\mu\} > 1$ there will be more than one state belonging to the representation $(\lambda\mu)$ with the same value of L. In a subsequent paper it is shown how the parameter K may be used to distinguish them. In fact they will be seen to arise from different intrinsic states, i.e. to belong to different bands.

To obtain the reduction of the irreducible representations [f] of U_s as representations of SU_3 the same technique as above may be used. Starting from the most simple representations and using the formulae for reducing product representations, the reduction of more complicated representations of U_s may be derived. Littlewood (1940, p 289) has discussed this general process, giving it the name plethysm. One is building tensors of symmetry [f] from single-particle functions which themselves transform as tensors of symmetry (NO) in the U_3 space. The problem is to determine according to which representation $(\lambda \mu)$ of U_3 these tensors of symmetry [f] transform. Calculations by Ibrahim (1950, 1952) provide the results necessary for determining which representations $(\lambda \mu)$ of SU_3 occur in a given representation [f] of SU_s . The range of his calculations cover most of the N=2 shell and the beginning of the N=3 shell.

6. The wave functions in the U_3 classification

The classification discussed in the last two sections was carried out in a rather abstract way. We dealt all the time with the quantum numbers $[f](\lambda\mu)L$ and made no use of the explicit form of the wave functions. In fact there is no need to derive their explicit forms. The concept of fractional parentage developed by Racah (1943) enables the antisymmetric k-particle functions to be defined in terms of the complete set of antisymmetric (k-1)-particle functions by a set of fractional parentage coefficients. Thus we can define and work with the states simply by knowing their fractional parentage coefficients. To calculate these coefficients we may again appeal to the rather abstract group-theoretical techniques used in the last two sections (see Racah 1951 for the general method). Calculation of these coefficients of fractional parentage is deferred until the third paper of this series where use is made of the rotational properties of the wave functions described in the second paper. However, it is instructive to study the explicit structure of the simple wave functions for two particles in an oscillator shell and we do that now.

In the oscillator shell with N=1 there is only a single orbital shell, the (1p) shell, and consequently no configuration mixing of the type considered here. The group U_3 is here identical with the full group U_s since s=(2l+1)=3. Thus the U_3 classification is identical with the supermultiplet classification and tells us nothing new about the states of the (1p) shell. A single 1p-particle has a single quantum of energy in the oscillator potential, its wave function transforming according to the representation (10) of SU_3 .

In the N=2 shell a single particle has two quanta of energy, its wave function transforming like a symmetric tensor of second rank in the space of SU_3 , being labelled by the representation (20). As may be seen from (14) this contains l-values of 0 and 2 corresponding to the orbital wave functions (2s) and (1d). With two particles in this shell there are two possible partitions [f], namely [2] and [11] corresponding to symmetric and antisymmetric orbital states respectively. The possible representations $(\lambda \mu)$ are given by the product

$$(20) \times (20) = (40) + (02) + (21),$$

which is similar to equation (11). This equation says that the product functions of the two particles transform under unitary transformations of SU_3 according to some mixture of the representations (40), (02) and (21). However, we may choose our functions such that they transform according to a particular one of these representations. The proof in § 3 that U_3 is a subgroup of U_s and contains R_3 as a subgroup means that we may so choose our functions without having to mix functions having different values of [f] or different values of L. From (14) the L-values contained in these representations ($\lambda\mu$) are as follows:

representation	dimension
(40) SDG	15
(02) SD	6
(21) PDF	15

The dimension check is also given. In this example it is simple to see which of these representations $(\lambda\mu)$ belong to the symmetric partition [2] and which to the antisymmetric partition [11] by appealing to the pure configurations. From the configurations s^2 , sd and d^2 with which we are concerned the only antisymmetric orbital states are P, D and an F state. Thus the reduction from [f] to $(\lambda\mu)$ must be as follows:

representation	dimension		
[2] (40) (02)	21		
[11] (21)	15		

Again we give the dimension check, the grand total being $36 = 6^2$, six being the number of single particle wave functions for the N = 2 shell.

In this example the two S-states are defined by the labels (40) S and (02) S instead of by definite configurations as d^2S and s^2S . They will be definite mixtures of these latter two states. To determine the coefficients in this mixture we must return to the group operators L_q and Q_q and use the property that the group operators cannot couple states belonging to different irreducible representations of U_3 . The G-state is unique so that the d^2G state is identical with the (40) G state. Now calculate the

matrix elements of Q_q between this G state and the two [2] D states defined by their configurations d^2 and ds. It then follows that the (02) D will be that combination of these two which has zero coupling with the (40) G state. The (40) D state then follows from orthogonality. By calculating the matrix element of Q_q between the (40) D state and the two S states defined by their configurations s^2 and d^2 we may in a similar way determine expressions for the (02) S and (40) S states in terms of those of a definite configuration. We find

$$\psi\{(40) S\} = \sqrt{\frac{5}{9}} \,\psi\{(s^2) S\} + \sqrt{\frac{4}{9}} \,\psi\{(d^2) S\},
\psi\{(40) D\} = \sqrt{\frac{7}{9}} \,\psi\{(ds) D\} - \sqrt{\frac{2}{9}} \,\psi\{(d^2) D\},$$
(15)

with orthogonal combinations for $\psi\{(02) S\}$ and $\psi\{(02) D\}$.

7. A comparison of the wave functions in the U_3 scheme with those of an energy calculation

So far we have derived a classification scheme on a purely mathematical basis. Such a scheme will be of practical use only if the wave functions so defined are close to those of the physical problem. For example the seniority classification (Flowers 1955) in j-j coupling is useful because it gives a good approximation to the wave functions of a pure configuration for very short range forces. The coupling schemes of this paper describe the mixing of configurations and so the wave functions must be compared with those of a shell-model energy calculation in which configuration mixing is taken into account. Such a calculation was made by Elliott & Flowers (1955) for two and three nucleons in the (1d) or (2s) shells. A comparison here is confused by the fact that the energy calculation was made in intermediate coupling whereas the U_3 scheme described here is only applicable to the L-S coupling extreme in its present form. Nevertheless, since the mode of intermediate coupling was near the L-S extreme a comparison here is still useful. It is found that the shell-model wave functions taken directly from the paper of Elliott & Flowers contain a very large proportion of the states classified according to the group U_3 and having the largest values for λ . Table 3 lists the states for which a comparison was made, giving in column three the appropriate label $(\lambda \mu)$ of the U_3 classification. Column five gives the percentage of intensity of these U_3 wave functions contained in the wave functions of the energy calculation. Although the percentages are all large some would be larger still but for the effect of intermediate coupling produced by the spin-orbit coupling. To illustrate this, column four gives the percentages of the wave functions from the energy calculation which belong to the lowest partition [f]. These figures are then an upper limit for the figures of column five.

To take the comparison further and to avoid the intermediate coupling effect, a calculation was made for the nucleus 20 Ne in L–S coupling but allowing full configuration mixing. With four particles in the (1d) or (2s) shells there are four S-states, five D-states, four G-states, etc., of the lowest partition [4]. The energy matrix for a Yukawa force was evaluated and diagonalized in the usual way to give a spectrum and wave functions. The exchange properties of the force are irrelevant in these states of full orbital symmetry [4], and since also S=0 for these states, we

have J=L. In table 3 we compare the lowest states of each spin from this calculation with those of the (80) representation in the U_3 scheme and they are seen to be very similar. The two figures of 100 % in column five are trivial because in those cases there is only one state with that value for L.

The calculated spectrum of these low states of ²⁰Ne is shown in Table 4 using the same interaction as in ¹⁹F (Elliott & Flowers 1955). The energy ratios are given and compared with those of the rotational model. Although close agreement is not found there is some similarity, and the order is correctly given. Some distortion of the

Table 3. A comparison between the wave functions of a standard shell model calculation and those of the U_3 scheme

$\operatorname{nucleus}$	${f T}$	J	$(\lambda \mu) L$	$\%(L\!-\!\!S)$	$\%(U_3)$	
$^{18}\mathrm{F}$	0	1	(40) S	97	92	ó
	0	3	(40) D	98	96	
	0	5	(40) G	100	100	(trivial)
18O	1	0	(40) S	86	72	•
	1	2	(40) D	80	72	•
$^{19}\mathrm{F}$	$\frac{1}{2}$	$\frac{1}{2}$	(60) S	92	92	•
	12 12 12 12	1 2 5 2 3 2 9 2	(60) D	86	74	•
	$\frac{1}{2}$	$\frac{3}{2}$	(60) D	84	74	
	$\frac{1}{2}$	$\frac{9}{2}$	(60) G	87	85	•
$^{20}{ m Ne}$	0	0	(80) S	100	92	•
	0	2	(80) D	100	99	•
	0	4	(80) G	100	92	•
	0	6	(80) I	100	99	. •
	0	8	(80) L	100	100	(trivial)

Table 4. A comparison between the $^{20}\mathrm{Ne}$ energy levels calculated in L--S coupling and those of a rotational K=0 band

J	0	2	f 4	6	8
$E({ m MeV})$	0	1.6	3.9	$7 \cdot 4$	10.3
ratios	0	1	$2 \cdot 4$	$4 \cdot 6$	$6 \cdot 4$
rotational ratios	0	1	$3 \cdot 3$	$7 \cdot 0$	12.0

rotational spectrum is to be expected here, related to the cutting off of the band at J=8. A true rotational band, for which the ratios are given, would continue indefinitely. The problem of the energy matrix will be discussed in the third paper of this series. It will be shown there that, if the interaction is of such a kind that, within an oscillator shell, the U_3 wave functions are exact, then the levels within a representation $(\lambda\mu)$ have an exactly rotational spectrum, with energies proportional to L(L+1). The relative position of states belonging to different representation $(\lambda\mu)$ is largely governed by the quantity $\lambda + \mu$ with the large values of $\lambda + \mu$ corresponding to low states.

There are two main factors determining the many-particle shell-model wave functions. One is the mixing of nearly degenerate configurations caused by the interparticle forces, and the other is the degree of intermediate coupling governed by the relative effectiveness of the inter-particle force and the spin-orbit force. The results presented in table 3 indicate that the classification of states by the group U_3 goes

a long way towards describing the mixing of configurations, at least in this particular mass-region. Before detailed comparison with experiment can be made, the effect of the spin-orbit force must be included. Since the U_3 scheme appears to describe the mixing of configurations so well it should be possible to carry out reliable intermediate coupling calculations throughout the (ds) shell with N=2, without too much labour, by selecting a limited number of the lowest U_3 states as a basis.

8. Conclusion

The general group-theoretical ideas of Racah have been used to derive classification schemes for particles in mixed orbital configurations. In particular, a scheme has been developed, using the group U_3 , for classifying the states of particles in a harmonic oscillator level, which has degenerate orbital states. The same group may be used for all the oscillator levels and may be looked upon as a generalization of the symmetry classification used in the (1p) shell.

The most interesting property of the classification is the association of states of different angular momenta in a way resembling that of a rotational band. The band is, however, cut off at some upper limit. In the second paper of this series we shall follow this lead and find the reason for the apparent band structure. The U_3 wave functions will be expressed as integrals over intrinsic states, thus demonstrating their rotational properties and showing that the U_3 coupling scheme is indeed a collective one.

The comparisons made in §7 between the U_3 wave functions and those of a straightforward shell-model calculation show a great similarity, indicating that the U_3 classification is physically important. It is found that the states with large values of $\lambda + \mu$ are lowest. This gives an interesting contrast with the seniority classification. There, the states of seniority zero or one are lowest, transforming like a scalar or a single particle wave function under the appropriate group. In the U_3 classification the states with largest values of $\lambda + \mu$ for a given number k of particles are lowest, and they are the most complicated functions. Such functions cannot be constructed with less than k particles. Thus we see that, whereas the seniority classification has some connexion with the single particle model, as is well known, the U_3 classification is more appropriate to a collective description in which all particles play an important part.

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Appendix. The R_6 classification for a mixed d and s shell

In the notation of § 2 the set of 36 operators for the full group U_6 of transformations in the six-dimensional space spanned by the single particle functions

$$\phi(dm), \phi(s0)$$
 $\mathbf{u}^{(0)}(ss), \mathbf{u}^{(0)}(dd),$
 $\mathbf{u}^{(1)}(dd),$
 $\mathbf{u}^{(2)}(sd), \mathbf{u}^{(2)}(ds), \mathbf{u}^{(2)}(dd),$
 $\mathbf{u}^{(3)}(dd),$
 $\mathbf{u}^{(4)}(dd),$

each tensor operator $\mathbf{u}^{(k)}$ having (2k+1) components $u_p^{(k)}$. The three operators $\mathbf{u}^{(1)}(dd)$ describe the rotation group R_3 , while the ten operators $\mathbf{u}^{(1)}(dd)$ and $\mathbf{u}^{(3)}(dd)$ describe the group R_5 . Including with these the five operators $\mathbf{u}^{(2)}(sd) + \mathbf{u}^{(2)}(ds)$ we may show from their commutators (4) that the set describes a group which may be identified with R_6 . This means that the orbital states may be simultaneously classified according to irreducible representations [f], (λ) , (σ) and L of the groups U_6 , R_6 , R_5 and R_3 .

The irreducible representations of R_6 are labelled by three integers $(\lambda) \equiv (\lambda_1 \lambda_2 \lambda_3)$ and the dimension of the representation is given by (Littlewood 1940, p. 236).

$$\tfrac{1}{6}(\lambda_1-\lambda_2+1)\left(\lambda_1-\lambda_3+2\right)\left(\lambda_2-\lambda_3+1\right)\left(\lambda_1+\lambda_2+3\right)\left(\lambda_1+\lambda_3+2\right)\left(\lambda_2+\lambda_3+1\right),$$

except for $\lambda_3 = 0$ when this value is halved. Using the reduction of product representations as in § 4 and in the paper by Jahn (1950), one may derive the classification given in table 5 for the lowest two supermultiplets of up to four nucleons in the combined d and s shell.

For two particles the two S states defined by their U_6 scheme are given by

$$\psi\{(000)(00)S\} = (\frac{1}{6})^{\frac{1}{2}}\psi\{(s^2)S\} + (\frac{5}{6})^{\frac{1}{2}}\psi(d^2)S\}$$

and its orthogonal partner

$$\psi\{(200)\,(00)\,S\} = (\frac{5}{6})^{\frac{1}{2}}\,\psi\{(s^2)\,S\} - (\frac{1}{6})^{\frac{1}{2}}\,\psi\{(d^2)\,S\},\,$$

while the two D states are still defined by their configurations,

$$\psi\{(200) (10) D\} = \psi\{(ds) D\},\$$

$$\psi\{(200) (20) D\} = \psi\{(d^2) D\}.$$

Although there is very little coupling between these two S-states for any reasonably short range interaction there always seems to be strong coupling between the two D-states, i.e. between the d^2 and ds configurations. For this reason it seems that this classification is not physically significant at the beginning of the nuclear (1d, 2s) just above ¹⁶0. It is clear from table 5 that the classification corresponds to a generalization of seniority to a mixed configuration in L-S coupling.

Table 5. The classification of the orbital states of the combined 1d and 2s shell using the groups $R_{\bf 6}$ and $R_{\bf 5}$

n	[<i>,f</i>]	$(\lambda_1\lambda_2\lambda_3)$	$(\sigma_1\sigma_2)$	L
0	[0]	(000)	(00)	S
			(00)	S
1	[1]	(100)	(10)	D
2	[2]	(000)	(00)	S
		, ,	(00)	S
		(200)	$\{(10)$	D
		` ,	(20)	DG
	£117	(110)	(10)	$oldsymbol{D}^+$
	[11]	(110)	(11)	PF
0	ro.,	(100)	$\hat{(00)}$	S
3	[3]	(100)	(10)	D
			(00)	${\mathcal S}$
		(200)	(10)	D
		(300)	(20)	DG
			(30)	SFGI
	re11	(100)	(00)	S
	[21]	(100)	(10)	D
			(10)	D
		(910)	(20)	DG
		(210)	$\tilde{1}(11)$	PF
			(21)	PDFGH
4	[4]	(000)	(00)	S
			(00)	S
		(200)	{(10)	D
			(20)	DG
			(00)	S
			(10)	D
		(400)	$\{(20)$	DG
		* '	(30)	SFGI
			(40)	DGHIL
			(00)	\underline{S}
	[31]	(200)	$\{(10)$	D
			(20)	DG
		(110)	$\{(10)$	D
		,	l(11)	PF
			$\binom{(10)}{(20)}$	D_{CC}
			(20)	DG
		(310)	$\int_{1}^{1} (11)$	PF
		, ,	(30)	SFGI
			(21)	$PDFGH \ PDF^2GH^2IK^2$
			(31)	LDE"GH"IK"