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GROUP THEORY OF HARMONIC OSCILLATORS

(III). States with Permutational Symmetry

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Abstract: This article continues the analysis of the problem of n particles in a common harmonic oscillator potential that was initiated in two previous papers under the same general title. The first objective of the paper is to give an analytic procedure for the explicit construction of the states in the $U_{3n} \supset \mathscr{U}_3 \times U_n$, $\mathscr{U}_3 \supset \mathscr{R}_3 \supset \mathscr{R}_2$, $U_n \supset U_{n-1} \supset \ldots \supset U_1$ chain of subgroups, where the $3n$ dimensional unitary group U_{3n} is the symmetry group of the Hamiltonian while $\mathscr{U}_3$ is the symmetry group of the harmonic oscillator, $\mathscr{R}_3$ is the ordinary rotation group, and U_n is the unitary group in n dimensions associated with the particle indices. The second and main objective of this paper is to construct states with definite permutational symmetry. After taking out the centre-of-mass motion the states given in terms of $n-1$ relative Jacobi vectors will be a basis for irreducible representations of the unitary group U_{n-1} and its orthogonal subgroup O_{n-1}. The characterization of the states is completed with the help of the irreducible representations of the symmetric group S_n, which, through its representations $D^{[n-1,\ 1]}(S_n)$, is a subgroup of O_{n-1}. This implies that the states transform irreducibly under the groups in the chain $U_n \supset U_{n-1} \supset O_{n-1} \supset S_n$ rather than under those in the chain $U_n \supset U_{n-1} \supset \ldots \supset U_1$. The states classified in this way contain as particular cases, those of both the shell and the cluster model. Explicit expressions are given for two, three and four particles.

1. Introduction

The present paper is a continuation of the two papers with the same general title by Bargmann and Moshinsky [1,2]) that will be denoted in what follows as BM I,II.

As indicated in BM I, this series will deal with the classification and determination of states of n particles when these particles move in a three-dimensional harmonic oscillator central potential. The main advantage of using a harmonic oscillator instead of an arbitrary common potential for the particles stems from the fact that in the former case the Hamiltonian is invariant under a unitary group in $3n$ dimensions [1-4]) U_{3n} while in the latter the Hamiltonian is invariant only under the direct product of the rotation group in three dimensions and the permutation group of n particles, i.e. $\mathscr{R}_3 \times S_n$. The group U_{3n} has as a subgroup [1-4]) the direct product of the unitary group in three dimensions $\mathscr{U}_3$ which is the symmetry group of the three dimensional harmonic oscillator [4]) and of the unitary group in n dimensions U_n associated with the particle indices [4]), i.e. $\mathscr{U}_3 \times U_n$. The group $\mathscr{U}_3$ has as a subgroup the rotation group [1-4]) $\mathscr{R}_3$, while U_n has as a subgroup the permutation group of n

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particles [2-4]) S_n, and so $\mathscr{U}_3 \times U_n$ contains in turn $\mathscr{R}_3 \times S_n$. This higher symmetry of the harmonic oscillator potential allows the development of very powerful techniques which have no counterpart for any other type of common potential [5]).

In particular in BMI, II a systematic technique is developed for the determination of a set of commuting integrals of motion invariant under $\mathscr{U}_3$ for a system of n particles in an harmonic oscillator. These integrals of motion, when supplemented with the orbital angular momentum and its projection, as well as with one operator more [1,2]) denoted by Ω, form a complete set and their corresponding eigenstates of highest weight in U_n were also determined in BM II. The states characterized by these integrals of motion will remain eigenstates when we add to our Hamiltonian a quadrupole-quadrupole interaction [1,2]) and so they already include the correlations associated with long range interactions [6]). These states were constructed in a synthetic way with the help of the special Wigner coefficients of $S\mathscr{U}_3$ obtained by one of the authors [7]).

The purpose of this paper is twofold. In the first place we want to give an analytic procedure for constructing our states starting with highest weight states in U_n of BM II, rather than by the synthetic procedure of ref. [7]). This will essentially involve characterizing the states by the canonical chain of subgroups $U_{n-1} \supset U_{n-2} \supset \ldots \supset U_1$ of U_n and determining these states from the highest state of U_n with the help of appropriate lowering operators [8]), all of which will be discussed in sect. 2.

The second purpose, and the main object of this paper, will be to construct states of definite permutational symmetry in configuration space so that, when they are combined with the appropriate spin-isospin states, the Pauli principle will be satisfied. This will involve the characterization of the states by the subgroup S_n of U_n rather than by the canonical chain of the previous paragraph. We shall first discuss in sect. 3 some general properties of the S_n group and its representations, and in sect. 4 the centre-of-mass motion before discussing the 2-, 3- and 4-particle problems in sects. 5 and 6, respectively. The four-particle case will be analysed in full details as it is already general enough to have all the features of the n-particle problem that will, in turn, be discussed in sect. 7.

As a systematic procedure of construction of spin-isospin states of definite permutational symmetry has been given in another paper [9]) we are in a position to discuss the complete n-nucleon problem in an harmonic oscillator without restricting ourselves to any particular shell. This provides us with states which include [4,10]) as particular cases, those of both the shell model and the cluster model [11]) and will allow us in future papers of this series to discuss the relations between these two models, as well as the group theoretical ideas underlying the clustering problem.

2. States Characterized by the Chain of Groups $U_{3n} \supset \mathscr{U}_3 \times U_n$

We shall keep the notation employed in BM I, II with the following changes: we denote by $\boldsymbol{x}^s$, $\boldsymbol{p}^s$ the coordinate and momentum vectors of particle s with components

$$\boldsymbol{x}^s = (x_1^s, x_2^s, x_3^s), \qquad s = 1, 2 \dots n, \tag{2.1}$$
$$\boldsymbol{p}^s = (p_1^s, p_2^s, p_3^s),$$

and consider n particles in a common harmonic oscillator potential with Hamiltonian

$$\mathscr{H} = \sum_{s=1}^{n} \sum_{j=1}^{3} \left(\frac{1}{2m} (p_j^s)^2 + \tfrac{1}{2} m\omega^2 (x_j^s)^2 \right), \tag{2.2}$$

where coordinates and momenta obey the canonical commutation relations.

On introducing

$$\boldsymbol{\eta}^s = \sqrt{\tfrac{1}{2}} \left(\sqrt{\frac{m\omega}{\hbar}}\, \boldsymbol{x}^s - i \sqrt{\frac{1}{m\omega\hbar}}\, \boldsymbol{p}^s \right),$$

$$\boldsymbol{\xi}^s = \sqrt{\tfrac{1}{2}} \left(\sqrt{\frac{m\omega}{\hbar}}\, \boldsymbol{x}^s + i \sqrt{\frac{1}{m\omega\hbar}}\, \boldsymbol{p}^s \right) = (\boldsymbol{\eta}^s)^\dagger, \tag{2.3}$$

we obtain

$$[\eta_j^s, \eta_k^t] = [\xi_j^s, \xi_k^t] = 0, \qquad [\xi_j^s, \eta_k^t] = \delta^{st} \delta_{jk}, \tag{2.4}$$

which allow us to interpret

$$\xi_j^s \equiv \frac{\partial}{\partial \eta_j^s}. \tag{2.5}$$

We introduce now the dimensionless Hamiltonian

$$H = \frac{1}{\hbar\omega} \mathscr{H} - \tfrac{3}{2} n = \sum_{s=1}^{n} \sum_{j=1}^{3} \eta_j^s \xi_j^s = \sum_{s=1}^{n} \sum_{j=1}^{3} \eta_j^s (\eta_j^s)^\dagger \tag{2.2'}$$

and see immediately that it is invariant under a $3n$ dimensional unitary transformation U_{3n} affecting the indices j, s of η_j^s.

The $(3n)^2$ operators

$$C_{jk}^{st} = \eta_j^s \xi_k^t, \qquad t, s = 1, 2 \dots n \qquad k, j = 1, 2, 3 \tag{2.6}$$

satisfy from (2.4) and (2.3) the relations

$$[C_{jk}^{st}, C_{j'k'}^{s't'}] = \delta^{ts'} \delta_{kj'} C_{jk'}^{st'} - \delta^{st'} \delta_{jk'} C_{j'k}^{s't}, \tag{2.7}$$

$$(C_{jk}^{st})^\dagger = C_{kj}^{ts}, \tag{2.8}$$

and so can be interpreted as the generators [2]) of the U_{3n} group. The invariance of the Hamiltonian (2.2') under U_{3n} implies that H commutes with all C_{jk}^{st} which we can also check independently using (2.4).

The generators of U_{3n} can be contracted either with respect to the upper or the lower indices giving the operators

$$\mathscr{C}_{jk} = \sum_{s=1}^{n} C_{jk}^{ss}, \qquad C^{st} = \sum_{j=1}^{3} C_{jj}^{st}. \tag{2.9a, b}$$

From (2.7) the 9 operators $\mathscr{C}_{jk}$ and n^2 operators C^{st} satisfy among themselves commutation relations [1,2]) and hermiticity conditions similar to those of the C^{st}_{jk}, and thus they are the generators of the unitary groups $\mathscr{U}_3$ and U_n, respectively. Besides,

$$[\mathscr{C}_{jk}, C^{st}] = 0, \tag{2.10}$$

and so these operators generate the subgroups $\mathscr{U}_3 \times U_n$ in the chain

$$U_{3n} \supset \mathscr{U}_3 \times U_n. \tag{2.11a}$$

The groups $\mathscr{U}_3$ and U_n are connected with the unitary transformations of η_j^s affecting respectively the indices $j = 1, 2, 3$ and $s = 1, 2, \ldots n$. These groups admit the canonical [12,13]) chain of subgroups

$$\mathscr{U}_3 \supset \mathscr{U}_2 \supset \mathscr{U}_1, \qquad U_n \supset U_{n-1} \supset \ldots \supset U_m \supset \ldots \supset U_1, \tag{2.11b, c}$$

where the group U_m, $m = 1, 2, \ldots n$ affects only the index s in η_j^s if s takes the values $s = 1, 2, \ldots m$, while $\mathscr{U}_3$, $\mathscr{U}_2$ and $\mathscr{U}_1$ affect only the indices $j = 1, 2, 3$, $j = 1, 2$ and $j = 1$, respectively. The generators of U_m, $m = 1, 2, \ldots n$, and of $\mathscr{U}_k$, $k = 1, 2, 3$, are respectively C^{st}, $1 \leqq s, t \leqq m$ and $\mathscr{C}_{ij}$, $1 \leqq i, j \leqq k$.

The eigenvalues [1]) of the Hamiltonian H are non-negative integers N, and the set of eigenstates corresponding to a given N could be characterized by the requirement that they form a basis for an irreducible representation [14]) (BIR) for U_{3n} and all the subgroups in the chain (2.11). We shall prove that this requirement completely defines the states.

The subgroup $\mathscr{U}_3 \times U_n$ is very important from a physical standpoint [4,2]) as it separates the behaviour of the states in three dimensional space from that related to the particle indices. The subgroups in the chain (2.11b, c) on the other hand, form a mathematically natural rather than physically significant chain of subgroups [15]). We show later how to pass from the simple eigenstates corresponding to the chain (2.11) to the eigenstates associated with more physically significant chains of subgroups.

To construct explicitly the states characterized by the chain of subgroups (2.11) we first recall [1,2]) that the eigenstates of H with eigenvalue N are given by homogeneous polynomials of degree N in the η_j^s, i.e. $P(\eta_j^s)$ acting on the ground state

$$|0\rangle = (\pi)^{-\frac{3}{4}n} \exp\left[-\frac{m\omega}{\hbar} \sum_{s=1}^{n} \sum_{j=1}^{3} (x_j^s)^2\right]. \tag{2.12}$$

If these states are characterized by the chain of subgroups (2.11), we have additional quantum numbers associated with the irreducible representations of the groups $\mathscr{U}_k$, $k = 1, 2, 3$ and U_m, $m = 1, 2, \ldots n$. As these irreducible representations are characterized by the partitions $[h_{1k} \ldots h_{kk}]$, $\{k_{1m} \ldots k_{mm}\}$, we see that we could denote the states by Gelfand patterns [16]) in $\mathscr{U}_3$ and U_n, i.e. by

$$|[h_{jk}], \{k_{lm}\}\rangle = P^{[h_{jk}], \{k_{lm}\}}(\eta_j^s)|0\rangle, \tag{2.13}$$

where $1 \leqq j \leqq k \leqq 3$, $1 \leqq l \leqq m \leqq n$.

To obtain the states (2.13) we recall the procedure by which one obtains the basis for an irreducible representation of the $\mathscr{R}_3 \supset \mathscr{R}_2$ chain of groups. First one determines the state of highest weight $|ll\rangle$ in the basis, i.e. the one satisfying

$$L_+|ll\rangle = 0, \qquad L_0|ll\rangle = l|ll\rangle, \tag{2.14}$$

and then one applies the lowering operator L_- to get the states

$$|lm\rangle = \left[\frac{(l-m)!}{(l+m)!(2l)!}\right]^{\frac{1}{2}}(L_-)^{l-m}|ll\rangle. \tag{2.15}$$

In a similar way, to determine the states (2.13), we first obtain the state of highest weight in the $\mathscr{U}_3 \times U_n$ group, for which the corresponding polynomial satisfies the equation [12])

$$\mathscr{C}_{ij}P = 0, \qquad 1 \leqq i < j \leqq 3, \qquad \mathscr{C}_{kk}P = h_k P, \qquad 1 \leqq k \leqq 3, \tag{2.16a, b}$$

$$C^{st}P = 0, \qquad 1 \leqq s < t \leqq n, \qquad C^{qq}P = k_{qn}P, \qquad 1 \leqq q \leqq n, \tag{2.16c, d}$$

in which, from (2.5), the operators $\mathscr{C}_{ij}$, C^{st} are interpreted as differential operators, and where for convenience we denote h_{i3} simply as h_i. As shown in ref. [12]), the system of equations (2.16) has a solution if and only if

$$h_i = k_{in} \qquad i = 1, 2. 3, \qquad k_{ln} = 0 \qquad 3 < l \leqq n, \qquad h_1 \geqq h_2 \geqq h_3 \geqq 0, \tag{2.17}$$

and in this case [1, 2, 12])

$$P^{[h_1h_2h_3]} = \mathscr{N}[h_1 h_2 h_3](\Delta_1^1)^{h_1-h_2}(\Delta_{12}^{12})^{h_2-h_3}(\Delta_{123}^{123})^{h_3}, \tag{2.18a}$$

with

$$\Delta_{j_1j_2\ldots j_r}^{s_1s_2\ldots s_r} = \sum_{\mathfrak{p}} (-1)^{\mathfrak{p}}\eta_{j_1}^{s_1}\eta_{j_2}^{s_2}\ldots\eta_{j_r}^{s_r}, \tag{2.18b}$$

where $\mathfrak{p}$ denotes a permutation of $(s_1 \ldots s_r)$ and $\mathscr{N}$ the normalization coefficient [7])

$$\mathscr{N}[h_1 h_2 h_3] = \left[\frac{(h_1-h_2+1)(h_1-h_3+2)(h_2-h_3+1)}{(h_1+2)!(h_2+1)!h_3!}\right]^{\frac{1}{2}}. \tag{2.18c}$$

As the representations $\{k_{lm}\}$ and $\{k_{lm-1}\}$ of the groups U_m and its subgroup U_{m-1} are related by the inequalities

$$k_{1m} \geqq k_{1m-1} \geqq k_{2m} \geqq k_{2m-1} \geqq \ldots \geqq k_{m-1\,m-1} \geqq k_{mm}, \tag{2.19}$$

we conclude from (2.17) that the states (2.13) have $k_{lm} = 0$ if $l > 3$.

To obtain now all the states (2.13) from the highest weight state $P^{[h_1h_2h_3]}|0\rangle$, we have to determine the lowering operators which will play, with respect to the $\mathscr{U}_3$ and U_n groups and their subgroups (2.11b,c), the same role as L_- for the $\mathscr{R}_3 \supset \mathscr{R}_2$ chain. This problem reduces to finding the operators that lower the irreducible vector spaces of U_{m-1} contained in an irreducible vector space of U_m. These operators were obtained by Nagel and Moshinsky [8]) and we shall give here their results particularized to our problem. As indicated in the previous paragraph, the representations of U_m and U_{m-1} for the states (2.13) are given by $\{k_{1m}k_{2m}k_{3m}\}$ and $\{k_{1m-1}k_{2m-1}k_{3m-1}\}$, respectively.

For convenience we denote the states of highest weight in all canonical subgroups [12, 13]) of U_{m-1} by

$$\left|\begin{matrix} k_{im} \\ k_{im-1} \end{matrix}\right\rangle,$$

where $i = 1, 2, 3$. Then the effect of a lowering operator L^{ml} in U_m will be

$$L^{ml}\left|\begin{matrix} k_{im} \\ k_{im-1} \end{matrix}\right\rangle \propto \left|\begin{matrix} k_{im} \\ k_{im-1}-\delta_{il} \end{matrix}\right\rangle, \tag{2.20}$$

in the same way that in the case of the R_3 group $L_-|lm\rangle \propto |lm-1\rangle$.

It is clear [12]) that an arbitrary state $\{k_{lm}\}$ could be obtained from the highest weight state in U_n with the help of the lowering operators L^{ml}, $1 \leqq l < m \leqq n$. In a similar way all states $[h_{ij}]$ could be derived from the highest weight state in $\mathscr{U}_3$ with the help of lowering operators $\mathscr{L}_{ki}$, $1 \leqq i < k \leqq 3$.

The explicit expressions for the operators L^{ml} are

$$\begin{aligned} L^{21} &= C^{21}, \\ L^{31} &= C^{31}E^{12}+C^{21}C^{32}, \\ L^{32} &= C^{32}, \end{aligned} \tag{2.21a}$$

$n \geqq 4$:

$$\begin{aligned} L^{n1} &= (C^{n1}E^{12}E^{23}+C^{21}C^{n2}E^{13}+C^{31}C^{n3}E^{12}+C^{21}C^{32}C^{n3})\prod_{\mu=4}^{n-1}E^{1\mu}, \\ L^{n2} &= (C^{n2}E^{23}+C^{32}C^{n3})\prod_{\mu=4}^{n-1}E^{2\mu}, \\ L^{n3} &= C^{n3}\prod_{\mu=4}^{n-1}E^{2\mu}, \end{aligned} \tag{2.21b}$$

where

$$E^{st} = C^{ss}-C^{tt}+t-s, \qquad \prod_{\mu=4}^{3}E^{s\mu} \equiv 1,$$

while for $\mathscr{L}_{ik}$, $1 \leqq i < k \leqq 3$ we have the same expressions as in (2.21) if we replace C^{st} by $\mathscr{C}_{ik}$. The general state $|[h_{ij}], \{k_{lm}\}\rangle$ can be written as

$$\begin{aligned} |[h_{ij}], \{k_{lm}\}\rangle = \mathscr{N}[h_{ij}]\prod_{p=2}^{3}\prod_{\mu=1}^{p-1}(\mathscr{L}_{p\mu})^{h_{\mu p}-h_{\mu p-1}} \\ \times \mathscr{N}\{k_{lm}\}\prod_{q=2}^{n}\prod_{\lambda=1}^{q-1}(L^{q\lambda})^{h_{\lambda q}-h_{\lambda q-1}}P^{[h_1h_2h_3]}|0\rangle, \end{aligned} \tag{2.22a}$$

where $P^{[h_1h_2h_3]}$ is given by (2.18a) and the normalization constants are

$$\mathcal{N}\{k_{lm}\} = \left[\prod_{s=2}^{n}\left(\prod_{\mu\geq\lambda=1}^{s-1}\frac{(k_{\lambda s-1}-k_{\mu s-1}+\mu-\lambda)!}{(k_{\lambda s}-k_{\mu s-1}+\mu-\lambda)!}\prod_{\mu>\lambda=1}\frac{(k_{\lambda s-1}-k_{\mu s}+\mu-\lambda-1)!}{(k_{\lambda s}-k_{\mu s}+\mu-\lambda-1)!}\right)\right]^{\frac{1}{2}} \tag{2.22b}$$

and similarly for $\mathcal{N}[h_{ij}]$ on replacing k_{lm} in (2.22b) by h_{lm} and n by 3.

The state (2.22a) is an eigenstate of the set of operators $(C^{11}, C^{22}, \dots C^{nn})$ with corresponding set of eigenvalues $(w_1, w_2, \dots, w_n)$, called the weight of the state, and given by

$$w_s = \sum_{l=1}^{s} k_{ls} - \sum_{l=1}^{s-1} k_{ls-1}\,. \tag{2.23}$$

We have proved that the chain of subgroups (2.11) completely characterizes the states of definite energy N, as was shown also by other authors [17, 18]. Furthermore we obtained explicitly these states from the highest weight state using an analytic procedure which employs the lowering operators of the unitary groups in the same way as the lowering operator L_- is employed for the $\mathcal{R}_3 \supset \mathcal{R}_2$ chain.

As mentioned above, our chain of subgroups (2.11b), while very natural from a mathematical standpoint, is not very significant physically. In a general physical situation we would add to our harmonic potential a residual interaction whose only symmetries would be those of the rotation group $\mathcal{R}_3$ and the permutation group S_n. Therefore, rather than use the canonical chain (2.11b,c), we should use the chain $\mathcal{U}_3 \supset \mathcal{R}_3 \supset \mathcal{R}_2$, $U_n \supset S_n$.

The polynomial corresponding to the highest weight state in U_n, i.e. that satisfies (2.16c, d), but characterized by the chain $\mathcal{U}_3 \supset \mathcal{R}_3$ rather than by $\mathcal{U}_3 \supset \mathcal{U}_2 \supset \mathcal{U}_1$ was obtained explicitly in BM II. Therefore the states characterized by the irreducible representations of the chain of subgroups

$$U_{3n} \supset \mathcal{U}_3 \times U_n, \qquad \mathcal{U}_3 \supset \mathcal{R}_3 \supset \mathcal{R}_2, \qquad U_n \supset U_{n-1} \supset \dots \supset U_1 \tag{2.24a, b, c}$$

could be obtained from the polynomial in eqs. (60), (70) of BM II by applying the operators L^{mk} of (2.21) as well as L_-. The corresponding states could be denoted by

$$|[h_1h_2h_3]\omega LM,\ \{k_{lm}\}\rangle, \tag{2.25}$$

where ω, L, M give the eigenvalues of the operators

$$\Omega = \sum_{i,j=1}^{3}(\mathcal{C}_{ij}+\mathcal{C}_{ji})L_iL_j, \qquad L^2 = \sum_{i=1}^{3}(L_i)^2, \qquad L_3, \tag{2.26a, b, c}$$

where

$$L_j = -i\sum_{k,l=1}^{3}\varepsilon_{jkl}\mathcal{C}_{kl}, \tag{2.26d}$$

and where, as indicated in (2.17) and (2.19), $k_{in} = h_n$, $i = 1, 2, 3$, $k_{lm} = 0$ for $l > 3$.

The states (2.25) are identical to those constructed synthetically in ref. [7]) using the

Wigner coefficient of $S\mathscr{U}_3$ as from the discussion in BM II one sees that the operators $H^{(p)}$, $\Gamma^{(p)}$, $\Delta^{(p)}$ $p = 1, 2, \ldots n$ defined there in terms of $\mathscr{C}_{ij}$ could be (because of the contractions over the indices $i, j = 1, 2, 3$) rewritten in terms of Casimir operators of first, second and third degree of U_p, and these operators would be diagonal with respect to states classified by the chain of groups (2.24c).

We have dealt therefore also with the chain of groups $\mathscr{U}_3 \supset \mathscr{R}_3 \supset \mathscr{R}_2$ which is part of the physically significant chain (2.24a, b). It remains for us to deal with the chain $U_n \supset S_n$, and this will be the objective of the following sections of this paper.

3. Permutational Symmetry

In this section we derive, for the group S_n, a projection technique involving only the characters and a ladder procedure for the determination of states with permutational symmetry, and apply it to obtain the permutational symmetry of the Jacobi vectors and of the generators of U_n.

We start by briefly recalling some properties of the symmetric group S_n as discussed, for example, in the book of Hamermesh [19]) referred to in what follows as H.

The group S_n is formed by all permutations of n letters. All elements of S_n may be generated by taking products of two generators A, B with relations [20])

$$A^n = (BA)^{n-1}, \qquad B^2 = (BA^{-j}BA^j)^2 = E, \qquad j = 2, 3, \ldots [\tfrac{1}{2}n], \tag{3.1}$$

where in cycle notation

$$A = (1, 2, \ldots, n), \qquad B = (1, 2). \tag{3.2}$$

Usually the $n-1$ transpositions $(m-1, m) = A^{2-m}BA^{m-2}$ are taken as basic elements. For an arbitrary representation it suffices to specify the matrices $D(A)$, $D(B)$ so that the usual specification of all the matrices $D(m-1, m)$ is clearly redundant·

An irreducible representation of S_n is characterized by a partition $[\lambda_1\lambda_2 \ldots \lambda_n]$ where $\sum_i \lambda_i = n$ and $\lambda_1 \geqq \lambda_2 \geqq \ldots \geqq 0$. The rows of this representation may be labelled by fixing the representation with partition $[\lambda_{lm}]$, $1 \leqq l \leqq m \leqq n-1$ for each canonical subgroup S_m related to letters $1, 2 \ldots m$ in the chain $S_n \supset S_{n-1} \supset \ldots \supset S_m \supset \ldots S_1$. The partitions in this chain are restricted [9]) by the conditions $\lambda_{lm} \geqq \lambda_{l\,m-1} \geqq \lambda_{l+1\,m}$ and $\lambda_{lm-1} = \lambda_{lm} - \delta_{l, r_m}$ where we use the notation $\lambda_l = \lambda_{ln}$. The collection of numbers $Y = (r_n r_{n-1} \ldots r_1)$ is the Yamanouchi [21]) symbol of the row which, in turn, corresponds to a standard Young tableau with letter m at the end of the r_mth row of the Young pattern $[\lambda_{lm}]$ of S_m.

A basis function of an irreducible representation of S_n may again be denoted by a Yamanouchi symbol. The effect of the transposition $(m-1, m)$ on a basis function ϕ is given by (H p. 221)

$$r_m = r_{m-1}:$$

$$(m-1, m)\phi(r_n \ldots r_m\, r_{m-1} \ldots r_1) = \phi(r_n \ldots r_m\, r_{m-1} \ldots r_1), \tag{3.3a}$$

$r_m \neq r_{m-1}$:

$$(m-1, m)\phi(r_n \ldots r_m r_{m-1} \ldots r_1) = \sigma_m \phi(r_n \ldots r_m r_{m-1} \ldots r_1) + \sqrt{1-(\sigma_m)^2}\phi(r_n \ldots r_{m-1} \ldots r_1), \tag{3.3b}$$

with

$$(\sigma_m)^{-1} = \lambda_{r_m m} - \lambda_{r_{m-1} m} + r_{m-1} - r_m.$$

We write (3.3b) as $r_m \neq r_{m-1}$:

$$\phi(r_n \ldots r_{m-1} r_m \ldots r_1) = \frac{1}{\sqrt{1-(\sigma_m)^2}}[(m-1, m) - \sigma_m]\phi(r_n \ldots r_m r_{m-1} \ldots r_1) \tag{3.4}$$

and note that, provided we know the effect of $(m-1, m)$, we may obtain by means of (3.4) new basis functions from a given one. In fact, since we can reach all basis functions by such transpositions, we may derive by a ladder procedure all basis functions from a single one which corresponds to the Young tableau with letter in natural order and which has the Yamanouchi symbol $Y = ((n)^{\lambda_n}(n-1)^{\lambda_{n-1}} \ldots 2^{\lambda_2}1^{\lambda_1})$.

We now want to construct basis functions for the irreducible representations of S_n from an arbitrary set of functions. The permutations $\mathfrak{p}$ act as operators when applied to the members of this set and with complex coefficients $f(\mathfrak{p})$ we form from them the elements

$$F = \sum_{\mathfrak{p} \in G} f(\mathfrak{p})\mathfrak{p} \tag{3.5}$$

of the algebra $\mathfrak{A}$ of the group [22] $G = S_n$ (H p. 108). Operators $\mathfrak{J}$ of $\mathfrak{A}$ which characterize in the same way all basis functions of a given irreducible representation of G, should commute with all group elements $\mathfrak{p}$. It follows that the operators $\mathfrak{J}$ are elements of a commutative subalgebra of $\mathfrak{A}$ called the central of $\mathfrak{A}$ and that their coefficients $i(\mathfrak{p})$ in $\mathfrak{J} = \sum_{\mathfrak{p}} i(\mathfrak{p})\mathfrak{p}$ are class functions [22] fulfilling $i(\mathfrak{p}\mathfrak{p}') = i(\mathfrak{p}'\mathfrak{p})$. The simplest elements of this type are the "sums of a class [24])" (SOC) defined by

$$\mathfrak{R}^{(k)} = \sum_{\mathfrak{p} \in k} \mathfrak{p}, \tag{3.6}$$

where k denotes a class of G, which clearly form [23] a basis of the central of $\mathfrak{A}$. They are the linearly independent operators $\mathfrak{J}$ which we are looking for. For a finite group G we may assume that the operators corresponding to the group elements $\mathfrak{p}$ are unitary. Consequently for all ambivalent classes (H p. 146) containing $\mathfrak{p}^{-1}$ together with $\mathfrak{p}$ the SOC are hermitian. Moreover, the SOC allow us to construct the basis functions of the irreducible representations of G by projection technique [24]. To see this we recall from the representation theory of finite groups that

$$\mathfrak{P}^\alpha = \frac{n_\alpha}{g} \sum_{\mathfrak{p} \in G} (\chi^\alpha(\mathfrak{p}))^* \mathfrak{p}, \tag{3.7}$$

n_α denoting the dimension of the irreducible representation α of G, $\chi^\alpha(\mathfrak{p})$ being the character of the element $\mathfrak{p}$, and g the order of G, are projection operators fulfilling

$$\mathfrak{P}^\alpha \mathfrak{P}^\beta = \delta^{\alpha\beta} \mathfrak{P}^\alpha. \tag{3.8}$$

Since the characters are class functions, we find

$$\mathfrak{P}^{\alpha} = \frac{n_{\alpha}}{g} \sum_{k} (\chi^{\alpha}(k))^{*} \mathfrak{K}^{(k)}, \tag{3.7'}$$

giving the projection operators in terms of the SOC for the irreducible representation α of G. If the elements $\mathfrak{p}$ are represented by unitary operators, it follows from $\chi^{\alpha}(\mathfrak{p}^{-1}) = (\chi^{\alpha}(\mathfrak{p}))^{*}$ and (3.7) that $\mathfrak{P}^{\alpha}$ is hermitian. With the help of the orthogonality relations of the characters we obtain

$$\mathfrak{K}^{(k)} = \sum_{\alpha} \frac{g_k}{n_{\alpha}} \chi^{\alpha}(k) \mathfrak{P}^{\alpha}, \tag{3.9}$$

giving the SOC in terms of the projection operators where g_k is the number of elements in class k. Consequently for all basis functions of an irreducible representation α o G the $\mathfrak{K}^{(k)}$ are diagonal with eigenvalue given by $(g_k/n_{\alpha})\chi^{\alpha}(k)$.

So far, our analysis applies to any finite group and has been used successfully in solid state physics [24]). In the symmetric group S_n we take now advantage of the canonical chain of subgroups $S_n \supset S_{n-1} \supset \ldots \supset S_1$ and definite SOC and projection operators for each canonical subgroup S_m with classes k_m. We replace the letters α, β by the partitions $[\lambda_{lm}]$ and define the projection operators

$$\mathfrak{P}^{[\lambda_{lm}]} = \frac{n_{[\lambda_{lm}]}}{m!} \sum_{k_m} \chi^{[\lambda_{lm}]}(k_m) \mathfrak{K}^{(k_m)}, \qquad 1 \leqq m \leqq n. \tag{3.10}$$

Then the operator

$$\mathfrak{P}^{(r_n r_{n-1} \ldots r_1)} = \mathfrak{P}^{[\lambda_{ln}]} \mathfrak{P}^{[\lambda_{ln-1}]} \ldots \mathfrak{P}^{[\lambda_{l1}]} \tag{3.11}$$

with $\lambda_{lm-1} = \lambda_{lm} - \delta_{lr_m}$ will project out a basis function Φ with Yamanouchi symbo $Y = (r_n r_{n-1} \ldots r_1)$. Once we obtain in this way the basis function with $Y = (n^{\lambda_n}(n-1)^{\lambda_{n-1}} \ldots 1^{\lambda_1})$, all other basis functions are conveniently derived from it by the ladder procedure (3.4). For the projection operators (3.10) we need the characters of the irreducible representations of $S_n, S_{n-1}, \ldots S_1$ which are known [25]) up to $n = 16$ and may be computed from the Frobenius formula (H p. 189) or by other methods [26]).

We return now to our set of states and first look into the permutational symmetry of the vectors $\boldsymbol{\eta}^s$ (or $\boldsymbol{\xi}^s$) and of the generators C^{st}.

The set of vectors $\boldsymbol{\eta}^s$ (or $\boldsymbol{\xi}^s$) under permutations transforms according to a reducible representation of S_n which is known to contain the irreducible representations $[n]+[n-1, 1]$. This can be seen explicitly from the properties of the Jacobi vectors $\dot{\boldsymbol{\eta}}^s$ given by

$$\dot{\boldsymbol{\eta}}^s = \sqrt{\frac{1}{s(s+1)}} \sum_{t=1}^{s} \boldsymbol{\eta}^t - \sqrt{\frac{s}{s+1}}\, \boldsymbol{\eta}^{s+1}, \qquad 1 \leqq s \leqq n-1, \tag{3.12}$$

$$\dot{\boldsymbol{\eta}}^n = \sqrt{\frac{1}{n}} \sum_{t=1}^{n} \boldsymbol{\eta}^t.$$

The transformation matrix is clearly real, orthogonal, and of determinant $+1$ so that it is an element of the subgroup R_n of U_n. Now $\dot{\eta}^n$ is invariant under permutations as it corresponds to the centre-of-mass vector. The permutation $(m-1, m)$ changes the vectors $\dot{\eta}^{m-2}$ and $\dot{\eta}^{m-1}$ into

$$(m-1, m)\dot{\eta}^{m-2} = \frac{1}{m-1}\dot{\eta}^{m-2} + \sqrt{1-\left(\frac{1}{m-1}\right)^2}\dot{\eta}^{m-1},$$

$$(m-1, m)\dot{\eta}^{m-1} = \sqrt{1-\left(\frac{1}{m-1}\right)^2}\dot{\eta}^{m-2} - \frac{1}{m-1}\dot{\eta}^{m-1}, \qquad m \geqq 3. \tag{3.13}$$

We compare this with the transformation of the basis functions for the irreducible representation $[n-1, 1]$ and obtain from (3.3)

$$[\lambda_{lm}] = [m-1, 1], \qquad (\sigma_m)^{-1} = -(m-1), \tag{3.14}$$

from which we conclude that the vectors $\dot{\eta}^s$, $1 \leqq s \leqq n-1$ correspond to the basis functions of this representation and may be characterized by Yamanouchi symbols as

$$[n-1, 1]: \qquad \dot{\eta}(1^{n-m-1}21^m) = \dot{\eta}^m, \qquad 1 \leqq m \leqq n-1,$$

$$[n]: \qquad \dot{\eta}(1^n) = \dot{\eta}^n. \tag{3.15}$$

From (3.13) we see that a permutation on $(\dot{\eta}^1\dot{\eta}^2 \ldots \dot{\eta}^{n-1})$ is represented by an orthogonal matrix in $n-1$ dimensions and so is contained in an orthogonal subgroup O_{n-1} of U_n.

We turn now to the generators $\dot{C}^{st} = \dot{\eta}^s \cdot \xi^t$ of U_n which transforms under S_n according to the inner product $([n-1, 1]+[n])\otimes([n-1, 1]+[n])$ given by (H p. 254)

$$[n]\otimes[n] = [n], \tag{3.16a}$$

$$[n]\otimes[n-1, 1] = [n-1, 1], \tag{3.16b}$$

$$[n-1, 1]\otimes[n-1, 1] = [n]+[n-1, 1]+[n-2, 2]+[n-2, 1, 1], \qquad n \geqq 4. \tag{3.16c}$$

We shall write now the real linear combinations of the generators corresponding to definite Yamanouchi symbols of irreducible representations of S_n. These linear combinations are determined up to an arbitrary multiplicative constant, which we fix up to a sign, by requiring that the sum of the square of the coefficients be 1. The properties of the Jacobi vectors (3.15) allow us immediately to make the identifications for the linear combinations containing the centre-of-mass vector which correspond to the inner products (3.16a, b):

$$[n]: \qquad \dot{C}_0(1^n) = \dot{C}^{nn}, \tag{3.17}$$

$$[n-1, 1]: \qquad \dot{C}_0(1^{n-s-1}21^s) = \dot{C}^{sn}, (\dot{C}^{sn})^\dagger, \qquad 1 \leqq s \leqq n-1. \qquad (3.18\text{a, b})$$

To distinguish them from the combinations appearing on the right hand side of (3.16c) we added to them an index 0.

From the first $n-1$ Jacobi vectors we find

$$[n]: \qquad \dot{C}(1^n) = \sum_{s=1}^{n-1} \dot{C}^{ss}. \tag{3.19}$$

We may, therefore, assume the remaining combinations to be traceless. The symmetric and antimetric parts of the $\dot{C}^{st}$, $1 \leqq s,\ t \leqq n-1$ transform among themselves under orthogonal transformations. Therefore we first consider the antimetric part which generates the rotation group R_{n-1},

$$\dot{A}^{st} = -i(\dot{C}^{st} - \dot{C}^{ts}), \qquad 1 \leqq s < t \leqq n-1. \tag{3.20}$$

These generators branch under R_{n-2} into

$$\{\dot{A}^{st}\}_{1 \leqq s < t \leqq n-1} \supset \{\dot{A}^{st}\}_{1 \leqq s < t \leqq n-2} + \{\dot{A}^{sn-1}\}_{1 \leqq s < n-1}.$$

Under S_{n-1} the generator $\dot{A}^{sn-1}$ transform among themselves according to $[n-2, 1]$. But from (3.13) we see that

$$(n-1, n)\dot{A}^{n-2,n-1} = -\dot{A}^{n-2,n-1},$$

and so we conclude that this generator belongs to the representation $[n-2, 1, 1]$ of S_n. From this we find, using the ladder procedure (3.4), the identification

$$\dot{A}(31^{n-s-2}21^s) = \sqrt{\tfrac{1}{2}}\dot{A}^{sn-1}, \qquad 1 \leqq s < n-1. \tag{3.21}$$

Now we may apply the same reasoning to the generators $\dot{A}^{st}$ which have indices $1 \leqq s < t \leqq n-2$ and continuing this argument we finally obtain

$$[n-2, 1, 1]: \qquad \dot{A}(1^{n-t-1}31^{t-s-1}21^s) = \sqrt{\tfrac{1}{2}}\dot{A}^{st}. \tag{3.22}$$

The symmetric and traceless part of the $\dot{C}^{st}$ must then contain bases for representations $[n-1, 1]$ and $[n-2, 2]$. We need the Clebsch-Gordan coefficients for these representations coupled from two representations $[n-1, 1]$. First we consider the coupling to $[n-1, 1]$ and therefore look for a combination of the generators $\dot{C}^{st}$ which transforms like $\dot{\eta}^{n-1}$ under permutations. Such an expression is found to be (appendix 1)

$$\dot{C}(21^{n-1}) = \sqrt{\frac{1}{(n-1)(n-2)}}\left(\sum_{s=1}^{n-2} \dot{C}^{ss} - (n-2)\dot{C}^{n-1\,n-1}\right),$$

in agreement with a result stated in (H p. 272). Now we apply the ladder procedure (3.4) to this expression and obtain

$$[n-1, 1]: \qquad \dot{C}(1^{n-s-1}21^s) = \sqrt{\frac{n}{n-2}}\left[\sqrt{\frac{1}{s(s+1)}}\left(\sum_{t=1}^{s-1} \dot{C}^{tt} - (s-1)\dot{C}^{ss}\right) + \sum_{t=s+1}^{n-1} \sqrt{\frac{1}{t(t+1)}}(\dot{C}^{st} + \dot{C}^{ts})\right], \qquad s \geqq 2 \tag{3.23a}$$

$$\dot{C}(1^{n-2}21) = \sqrt{\frac{n}{n-2}} \sum_{t=2}^{n-1} \sqrt{\frac{1}{t(t+1)}} (\dot{C}^{1t}+\dot{C}^{t1}). \tag{3.23b}$$

Finally we only state the result for the representation $[n-2, 2]$. We find (appendix 1)

$$[n-2, 2]: \qquad \dot{C}(221^{n-2}) = \frac{1}{n-2} \sqrt{\frac{1}{(n-1)(n-3)}} \Big[\sum_{t=1}^{n-3} \dot{C}^{tt}$$
$$-(n-3)\dot{C}^{n-2\,n-2} - \tfrac{1}{2}(n-3)\sqrt{n(n-2)}(\dot{C}^{n-1\,n-2}+\dot{C}^{n-2\,n-1})\Big] \tag{3.24}$$

and obtain the other partners by the ladder procedure, finding for example,

$$[n-2, 2]: \qquad \dot{C}(1^{n-s-2}221^{s}) = \frac{1}{s} \sqrt{\frac{1}{(s+1)(s-1)}} \Big[\sum_{t=1}^{s-1} \dot{C}^{tt}$$
$$-(s-1)\dot{C}^{ss} - \tfrac{1}{2}(s-1)\sqrt{s(s+2)}(\dot{C}^{ss+1}+\dot{C}^{s+1s})\Big], \qquad s \geqq 2. \tag{3.25}$$

The irreducible representations of S_n which we discussed are orthogonal. Therefore for any basis ϕ_i, $i = 1 \ldots n_{[\lambda]}$, the expression $\sum_{i=1}^{n[\lambda]} \phi_i \phi_i$ will be invariant under permutations. The results obtained in the last part of this section allow us then to form operators quadratic in the generators $\dot{C}^{st}$ which are invariant under permutation like, for example, the Casimir operator $\dot{\Lambda}^2 = \sum_{s<t}(\dot{\Lambda}^{st})^2$ of the orthogonal subgroup O_{n-1} of U_n. Operators with this property will help us to characterize states with permutational symmetry. We could also, using the Clebsch-Gordan coefficients of S_n, construct operators invariant under permutations of order higher than two in the generators.

4. Centre-of-Mass Motion

The Hamiltonian (2.2) is not translationally invariant. We could consider instead the translationally invariant Hamiltonian

$$\bar{\mathscr{H}} = \sum_{s=1}^{n} \frac{1}{2m} (\boldsymbol{p}^s)^2 + \frac{m\omega^2}{4n} \sum_{s,t=1}^{n} (\boldsymbol{x}^s - \boldsymbol{x}^t)^2 \tag{4.1}$$

and introduce Jacobi coordinates $\dot{\boldsymbol{x}}^s$ by

$$\dot{\boldsymbol{x}}^s = \sqrt{\frac{1}{s(s+1)}} \sum_{t=1}^{s} \boldsymbol{x}^t - \sqrt{\frac{s}{s+1}}\, \boldsymbol{x}^{s+1}, \qquad 1 \leqq s \leqq n-1,$$
$$\dot{\boldsymbol{x}}^n = \sqrt{\frac{1}{n}} \sum_{t=1}^{n} \boldsymbol{x}^t, \tag{4.2}$$

which have the property $\sum_{s=1}^{n}(\dot{\boldsymbol{x}}^s \cdot \dot{\boldsymbol{x}}^s) = \sum_{s=1}^{n}(\boldsymbol{x}^s \cdot \boldsymbol{x}^s)$. Consequently

$$\sum_{s,t=1}^{n} (\boldsymbol{x}^s - \boldsymbol{x}^t)^2 = 2n \sum_{s=1}^{n} (\dot{\boldsymbol{x}}^s)^2 - 2(\sum_{s=1}^{n} \boldsymbol{x}^s)^2 = 2n \sum_{s=1}^{n-1} (\dot{\boldsymbol{x}}^s)^2, \tag{4.3}$$

so that the Hamiltonian (4.1) becomes

$$\overline{\mathscr{H}} = \sum_{s=1}^{n} \frac{1}{2m} (\dot{\boldsymbol{p}}^s)^2 + \tfrac{1}{2} m\omega^2 \sum_{s=1}^{n-1} (\dot{\boldsymbol{x}}^s)^2. \tag{4.1'}$$

Comparing with (2.2) we obtain

$$\overline{\mathscr{H}} = \mathscr{H} - \tfrac{1}{2} m\omega^2 (\dot{\boldsymbol{x}}^n)^2. \tag{4.4}$$

Whereas $\overline{\mathscr{H}}$ allows for a translation of the centre of mass described by a plane wave $\exp\{i\boldsymbol{x}^n \cdot \boldsymbol{p}^n\}$, $\mathscr{H}$ contains possible excitations of the centre-of-mass vector. However, spurious states arise only if we consider states with different excitation of the centre-of-mass vector. Since the actual dependency of the states on $\dot{\boldsymbol{x}}^n$ is unessential, provided it is fixed for all states, we keep the original Hamiltonian (2.2) and avoid spurious states by giving no excitation to the centre-of-mass vector.

5. States with Permutational Symmetry for Two and Three Particles

We replace in the rest of the paper the ket notation (2.25) of the states by a bracket expression

$$\langle \boldsymbol{\eta} | [h_1 h_2 h_3] \omega LM, \{k_{lm}\} \rangle \tag{2.25'}$$

similar to the one employed by Dirac as this would allow us to differentiate the states in terms of the vectors $\boldsymbol{\eta} = \{\boldsymbol{\eta}^s\}$ related to the individual particles from any other linear combinations of the $\boldsymbol{\eta}^s$ suitable for our purpose.

In this section we examine states of two and of three particles. The four particles states which have already all the features of the n-particle case will be discussed in the following sect. 6.

(i) For two particles we obtain from $U_6 \supset \mathscr{U}_3 \times U_2$ the states

$$\left\langle \dot{\boldsymbol{\eta}}^1 \dot{\boldsymbol{\eta}}^2 \middle| [h_1 h_2 0] \omega LM, \begin{matrix} h_1 & & h_2 \\ & r_1 & \end{matrix} \right\rangle,$$

where

$$\begin{aligned} \dot{\boldsymbol{\eta}}^1 &= \sqrt{\tfrac{1}{2}} (\boldsymbol{\eta}^1 - \boldsymbol{\eta}^2), \\ \dot{\boldsymbol{\eta}}^2 &= \sqrt{\tfrac{1}{2}} (\boldsymbol{\eta}^1 + \boldsymbol{\eta}^2). \end{aligned} \tag{5.1}$$

If we eliminate centre-of-mass motion, we must have that the eigenvalue of $\dot{C}^{22}$ is zero, which implies we must have $h_1 + h_2 - r_1 = 0$. This leads to $h_2 = 0$, $r_1 = h_1$ so that $\dot{w}_1 = h_1$. From $(1,2)\dot{\boldsymbol{\eta}}^1 = -\dot{\boldsymbol{\eta}}^1$ we conclude that

$$(1,2) \left\langle \dot{\boldsymbol{\eta}}^1 \dot{\boldsymbol{\eta}}^2 \middle| [h_1 00] LM, \begin{matrix} h_1 & & 0 \\ & h_1 & \end{matrix} \right\rangle = (-1)^{h_1} \left\langle \dot{\boldsymbol{\eta}}^1 \dot{\boldsymbol{\eta}}^2 \middle| [h_1 00] LM, \begin{matrix} h_1 & & 0 \\ & h_1 & \end{matrix} \right\rangle, \tag{5.2}$$

which completely defines the permutational symmetry of the states. Their Yamanouchi symbol is $Y = (21)$ for h_1 even and $Y = (11)$ for h_1 odd.

(ii) For three particles [27]) we have Jacobi vectors

$$\begin{aligned} \dot{\eta}^1 &= \sqrt{\tfrac{1}{2}}(\eta^1-\eta^2), \\ \dot{\eta}^2 &= \sqrt{\tfrac{1}{6}}(\eta^1+\eta^2)-\sqrt{\tfrac{2}{3}}\eta^3, \\ \dot{\eta}^3 &= \sqrt{\tfrac{1}{3}}(\eta^1+\eta^2+\eta^3). \end{aligned} \tag{5.3}$$

We eliminate the centre-of-mass motion and obtain in $U_9 \supset \mathscr{U}_3 \supset U_3$ the states

$$\left\langle \dot{\eta}^1\dot{\eta}^2\dot{\eta}^3 \middle| [h_1 h_2 0]\omega LM, \begin{matrix} h_1 & h_2 & 0 \\ h_1 & h_2 & \\ & r_1 & \end{matrix} \right\rangle . \tag{5.4}$$

The permutations affect only the subgroup U_2 related to $\dot{\eta}^1$ and $\dot{\eta}^2$. From the permutational symmetry of the vectors $\dot{\eta}(211) = \dot{\eta}^2$, $\dot{\eta}(121) = \dot{\eta}^1$ we find the symmetries of the generators under S_3:

$$\begin{aligned} \dot{C}(111) &= \dot{C}^{11}+\dot{C}^{22}, \\ \dot{C}(121) &= \dot{F}^1 \equiv \tfrac{1}{2}(\dot{C}^{12}+\dot{C}^{21}), \\ \dot{C}(321) &= \dot{F}^2 \equiv -\tfrac{1}{2}i(\dot{C}^{12}-\dot{C}^{21}), \\ \dot{C}(211) &= \dot{F}^3 \equiv \tfrac{1}{2}(\dot{C}^{11}-\dot{C}^{22}), \end{aligned} \tag{5.5}$$

where $\dot{F}^1$, $\dot{F}^2$, $\dot{F}^3$ have the properties of the components of the pseudospin (BM I, II) of the group SU_2. Clearly $(\dot{F}^2)^2$ is invariant under permutations. Since it is, on the otherhand, the Casimir operator of the subgroup R_2 of SU_2, it is convenient to use the states in the chain $U_2 \supset R_2$ by diagonalizing $\dot{F}^2$. For this we introduce new coordinates

$$\begin{aligned} \ddot{\eta}^1 &= \sqrt{\tfrac{1}{2}}(-i\dot{\eta}^1+\dot{\eta}^2), \\ \ddot{\eta}^2 &= \sqrt{\tfrac{1}{2}}(i\dot{\eta}^1+\dot{\eta}^2), \\ \ddot{\eta}^3 &= \dot{\eta}^3, \end{aligned} \tag{5.6}$$

and consider states

$$\left\langle \ddot{\eta}^1\ddot{\eta}^2\ddot{\eta}^3 \middle| [h_1 h_2 0]\omega LM, \begin{matrix} h_1 & h_2 & 0 \\ h_1 & h_2 & \\ & r_1 & \end{matrix} \right\rangle . \tag{5.7}$$

Instead of h_1, h_2, r_1 we use

$$N = h_1+h_2, \qquad f = \tfrac{1}{2}(h_1-h_2), \qquad g = r_1-\tfrac{1}{2}(h_1+h_2), \tag{5.8}$$

which determine the energy, the square of the pseudospin and its component $\ddot{F}^3 = \dot{F}^2$. From the simple type of lowering operator (2.21) we obtain, for the state of highest weight in $\mathscr{U}_3$,

$$\begin{aligned} \langle \ddot{\eta} | Nfg \rangle &= \mathscr{N}(Nfg)(\ddot{\eta}_1^1)^{f+g}(\ddot{\eta}_1^2)^{f-g}(\ddot{\Delta}_{12}^{12})^{\frac{1}{2}N-f}, \\ \mathscr{N}(Nfg) &= \left[\frac{(2f+1)!}{(\frac{1}{2}N+f+1)!(\frac{1}{2}N-f)!(f+g)!(f-g)!}\right]^{\frac{1}{2}}. \end{aligned} \tag{5.9}$$

Now we note that the cyclic permutation $(1, 2, 3) = (2, 3)(1,2)$ acts on $\dot{\boldsymbol{\eta}}^1, \dot{\boldsymbol{\eta}}^2$ as

$$(1, 2, 3)\begin{pmatrix}\dot{\boldsymbol{\eta}}^1\\ \dot{\boldsymbol{\eta}}^2\end{pmatrix} = \begin{pmatrix}\cos\frac{2}{3}\pi & \sin\frac{2}{3}\pi\\ -\sin\frac{2}{3}\pi & \cos\frac{2}{3}\pi\end{pmatrix}\begin{pmatrix}\dot{\boldsymbol{\eta}}^1\\ \dot{\boldsymbol{\eta}}^2\end{pmatrix}. \tag{5.10}$$

Therefore we find for the vectors $\ddot{\boldsymbol{\eta}}^1, \ddot{\boldsymbol{\eta}}^2$

$$(1, 2, 3)\begin{pmatrix}\ddot{\boldsymbol{\eta}}^1\\ \ddot{\boldsymbol{\eta}}^2\end{pmatrix} = \begin{pmatrix}\exp(-\frac{2}{3}\pi i) & 0\\ 0 & \exp(\frac{2}{3}\pi i)\end{pmatrix}\begin{pmatrix}\ddot{\boldsymbol{\eta}}^1\\ \ddot{\boldsymbol{\eta}}^2\end{pmatrix}, \tag{5.11a}$$

$$(1, 2)\begin{pmatrix}\ddot{\boldsymbol{\eta}}^1\\ \ddot{\boldsymbol{\eta}}^2\end{pmatrix} = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\ddot{\boldsymbol{\eta}}^1\\ \ddot{\boldsymbol{\eta}}^2\end{pmatrix}. \tag{5.11b}$$

Then, adopting the standard notation of representations, we have from (5.9)

$$(1, 2, 3)\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle = \langle(1, 2, 3)^{-1}\ddot{\boldsymbol{\eta}}|Nfg\rangle = \exp(\tfrac{1}{3}\pi i2g)\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle, \tag{5.12a}$$

$$(1, 2)\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle = \langle(1, 2)^{-1}\ddot{\boldsymbol{\eta}}|Nfg\rangle = (-1)^{\frac{1}{2}N-f}\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle. \tag{5.12b}$$

We apply now the projection technique developed in sect. 3 and first write the SOC (3.6) of S_3 for the classes † with cycle length (1^3), (21) and (3)

$$\begin{aligned}\mathfrak{K}^{(1^3)} &= e,\\ \mathfrak{K}^{(21)} &= (1, 2)+(1, 3)+(2, 3) = (1, 2)+(1, 2)(1, 2, 3)+(1, 2, 3)(1, 2),\\ \mathfrak{K}^{(3)} &= (1, 2, 3)+(3, 2, 1) = (1, 2, 3)+(1, 2)(1, 2, 3)(1, 2).\end{aligned} \tag{5.13}$$

By means of the characters of S_3 (H p. 276) we obtain for the projection operators (3.7′)

$$\begin{aligned}\mathfrak{P}^{[3]} &= \tfrac{1}{6}[\mathfrak{K}^{(1^3)}+\mathfrak{K}^{(21)}+\mathfrak{K}^{(3)}],\\ \mathfrak{P}^{[2,1]} &= \tfrac{1}{3}[2\mathfrak{K}^{(1^3)}-\mathfrak{K}^{(3)}],\\ \mathfrak{P}^{[1^3]} &= \tfrac{1}{6}[\mathfrak{K}^{(1^3)}-\mathfrak{K}^{(21)}+\mathfrak{K}^{(3)}].\end{aligned} \tag{5.14}$$

First we look for the basis of the [2, 1] representation and find on applying $\mathfrak{P}^{[2,1]}$ to the states (5.9)

$$\mathfrak{P}^{[2,1]}\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle = \tfrac{1}{3}\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle[2-\exp(\tfrac{1}{3}\pi i2g)-\exp(-\tfrac{1}{3}\pi i2g)]. \tag{5.15}$$

We introduce ν by $2g \equiv \nu \bmod 3$, $\nu = 0,1,2$ and have

$$\mathfrak{P}^{[2,1]}\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle = \langle\ddot{\boldsymbol{\eta}}|Nfg\rangle[1-\delta_{\nu 0}]. \tag{5.16}$$

Now we apply the projection operator $\mathfrak{P}^{[2]} = \frac{1}{2}(e+(1, 2))$ in S_2 and obtain the basis function with $Y = (211)$ for $\nu = 1, 2$, $g > 0$

$$\phi(211) = \mathfrak{P}^{[2]}\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle = \tfrac{1}{2}[\langle\ddot{\boldsymbol{\eta}}|Nfg\rangle+(-1)^{\frac{1}{2}N-f}\langle\ddot{\boldsymbol{\eta}}|Nf-g\rangle]. \tag{5.17a}$$

In order to find the partner function with $Y = (121)$, we use the ladder procedure

† We shall distinguish between classes and permutations by using commas in the latter case, for example (3,1) is a transposition while (31) is a class.

(3.4) which yields

$$\phi(121) = \sqrt{\tfrac{4}{3}}[(2,3)+\tfrac{1}{2}]\phi(211),$$

and find for $\nu = 1{,}2,\ g > 0$

$$\phi(121) = \tfrac{1}{2}i(-1)^{\nu+1}[\langle \ddot{\boldsymbol{\eta}}|Nfg\rangle - (-1)^{\frac{1}{2}N-f}\langle \ddot{\boldsymbol{\eta}}|Nf-g\rangle]. \tag{5.17b}$$

In a similar way we obtain for the representation [3] if $\nu = 0,\ g > 0$

$$\langle \ddot{\boldsymbol{\eta}}|Nfg(111)\rangle = \sqrt{\tfrac{1}{2}}[\langle \ddot{\boldsymbol{\eta}}|Nfg\rangle + (-1)^{\frac{1}{2}N-f}\langle \ddot{\boldsymbol{\eta}}|Nf-g\rangle], \tag{5.18}$$

and for $[1^3]$ if $\nu = 0,\ g > 0$

$$\langle \ddot{\boldsymbol{\eta}}|Nfg(321)\rangle = \sqrt{\tfrac{1}{2}}[\langle \ddot{\boldsymbol{\eta}}|Nfg\rangle - (-1)^{\frac{1}{2}N-f}\langle \ddot{\boldsymbol{\eta}}|Nf-g\rangle], \tag{5.19}$$

and finally if $g = 0$ we see from (5.12b) that this state belongs to [3] or $[1^3]$ if $\frac{1}{2}(N-2f)$ is even or odd respectively.

We now go back to Jacobi vectors $\dot{\boldsymbol{\eta}}$ and write (5.6) in the usual Euler angle parametrization [28]) plus a phase δ, $-\pi < \delta \leqq \pi$,

$$(\ddot{\boldsymbol{\eta}}^1, \ddot{\boldsymbol{\eta}}^2) = (\dot{\boldsymbol{\eta}}^1, \dot{\boldsymbol{\eta}}^2)e^{i\delta}\begin{pmatrix} \cos\frac{\beta}{2}\exp\left(i\frac{\alpha+\gamma}{2}\right), & \sin\frac{\beta}{2}\exp\left(i\frac{\alpha-\gamma}{2}\right) \\ -\sin\frac{\beta}{2}\exp\left(i\frac{\gamma-\alpha}{2}\right), & \cos\frac{\beta}{2}\exp\left(-i\frac{\alpha+\gamma}{2}\right) \end{pmatrix}, \tag{5.6'}$$

with $\alpha = \frac{1}{2}\pi$, $\beta = \frac{1}{2}\pi$, $\gamma = \pi$, $\delta = \frac{3}{4}\pi$. Then, from the fact that the states transform according to irreducible representations of SU_2, it follows that

$$\langle \ddot{\boldsymbol{\eta}}|Nfg\rangle = \exp\left(\tfrac{3}{4}\pi iN\right)\sum_{g'}\langle \dot{\boldsymbol{\eta}}|Nfg'\rangle D^f_{g'g}(\tfrac{1}{2}\pi\tfrac{1}{2}\pi\pi), \tag{5.20}$$

where D^f denotes the representation matrix of SU_2 in the notation of Edmonds [28]).

We could easily express these states in terms of the $\boldsymbol{\eta}^s$, but in the applications of the present developments we would like to eliminate spurious states associated with centre-of-mass excitation. Therefore it is very convenient to express all results in terms of relative vectors such as for example, the Jacobi ones.

6. Four-Particle States with Permutational Symmetry

For four particles we have the Jacobi vectors

$$\begin{aligned} \dot{\boldsymbol{\eta}}^1 &= \sqrt{\tfrac{1}{2}}(\boldsymbol{\eta}^1-\boldsymbol{\eta}^2), \\ \dot{\boldsymbol{\eta}}^2 &= \sqrt{\tfrac{1}{6}}(\boldsymbol{\eta}^1+\boldsymbol{\eta}^2)-\sqrt{\tfrac{2}{3}}\boldsymbol{\eta}^3, \\ \dot{\boldsymbol{\eta}}^3 &= \sqrt{\tfrac{1}{12}}(\boldsymbol{\eta}^1+\boldsymbol{\eta}^2+\boldsymbol{\eta}^3)-\sqrt{\tfrac{3}{4}}\boldsymbol{\eta}^4, \\ \dot{\boldsymbol{\eta}}^4 &= \sqrt{\tfrac{1}{4}}(\boldsymbol{\eta}^1+\boldsymbol{\eta}^2+\boldsymbol{\eta}^3+\boldsymbol{\eta}^4) \end{aligned} \tag{6.1}$$

and the groups $U_{12} \supset \mathscr{U}_3 \times U_4$. We again eliminate the centre-of-mass motion so that U_4 reduces essentially to U_3. To see now what subgroups of U_3 are convenient to choose so as to have complete classification of states with permutational symmetry, we notice that the Jacobi vectors (6.1) transform under permutations according to the representation $D^{[3,1]}(S_4)$. As this representation is given by three dimensional orthogonal matrices, we see that it constitutes a subgroup of the O_3 group. Therefore it is convenient in the first place, to characterize the states by the chain of subgroups $U_3 \supset R_3 \supset R_2$ as $O_3 = R_3 \times \mathfrak{J}$ with $\mathfrak{J}$ being the inversion group, and our states under inversion I are multiplied by $(-1)^\kappa$, where

$$N = h_1 + h_2 + h_3 \equiv \kappa \bmod 2, \qquad \kappa = 0, 1. \tag{6.2}$$

In the case of $\mathcal{U}_3 \supset \mathcal{R}_3 \supset \mathcal{R}_2$ the states are completely characterized by the quantum numbers (ω, L, M) so that in a similar fashion, the states in the chain $U_3 \supset R_3 \supset R_2$ could be characterized by (φ, λ, μ).

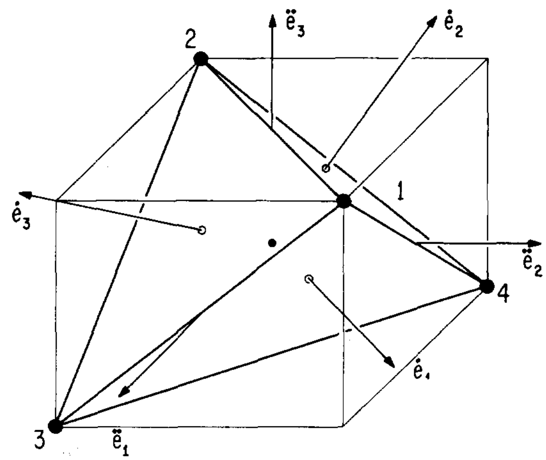

Fig. 1. Tetrahedron showing isomorphism between the group T_d of its symmetry operations and the permutation group S_4 on four objects 1, 2, 3, 4. Two systems of coordinates, $\dot{S} = (\dot{e}_1\dot{e}_2\dot{e}_3)$ and $\ddot{S} = (\ddot{e}_1\ddot{e}_2\ddot{e}_3)$, are used in the text.

We now restrict the operations O_3 to the transformations $D^{[3,1]}(S_4)$ of the Jacobi vectors under S_4. Let us refer these transformations for the moment to ordinary three-dimensional space. What, then, are the transformations $D^{[3,1]}(S_4)$ in this space? The answer is that they are in a one-to-one correspondence to the elements of the symmetry group T_d of a regular tetrahedron as is evident from fig. 1. The analysis of Coxeter and Todd [20]) shows, moreover, that there is, in general, an isomorphism between S_n and the symmetry operations of a regular simplex in $n-1$ dimensions. The fact that the chain $O_3 \supset T_d$ has been studied in detail [29,30]) for the analysis of the CH_4 molecular spectrum enables us to carry over the results from T_d to the isomorphic group S_4. From the comparison of the character tables of S_4(H p. 276) and

T_d (H p. 127) we have the correspondence between the classes and the irreducible representations given in table 1.

(a) The first point in our analysis will be to find, in general, the irreducible representations of $S_4 \approx T_d$ in a given representation of O_3. We denote the irreducible

TABLE 1

Characters of the isomorphic groups S_4 and T_d showing correspondence between classes and representations

		Class				
	T_d	(S_4)	(C_3)	$(S_4{}^2)$	(σ_d)	(E)
	S_4	(4)	(31)	(2^2)	(21^2)	(1^4)
Representation						
T_d	S_4					
A_1	$[4]$	1	1	1	1	1
F_2	$[3,1]$	-1	0	-1	1	3
E	$[2,2]$	0	-1	2	0	2
F_1	$[2,1^2]$	1	0	-1	-1	3
A_2	$[1^4]$	-1	1	1	-1	1
g_k		6	8	3	6	1
θ_k		$\mp\frac{1}{2}\pi$	$\pm\frac{2}{3}\pi$	π	π	0
$\psi^{0\lambda}$		$(-1)^\nu$	$1-\sigma$	$(-1)^\rho$	$(-1)^\rho$	$2\lambda+1$
$\psi^{1\lambda}$		$-(-1)^\nu$	$1-\sigma$	$(-1)^\rho$	$-(-1)^\rho$	$2\lambda+1$

The notation for classes and representations is taken from H p. 276 and p. 127, respectively. In the table, g_k is the number of elements in class k of S_4, θ_k is the rotation angle for the elements of class k [29]), and $\psi^{\kappa\lambda}(k)$ is the character of $D^{\kappa\lambda}(O_3)$ for $O_3 = D^{[3,1]}(k)$ in terms of ν, ρ, σ defined by $\lambda = 2\nu+\rho \equiv \rho \bmod 2$, $\lambda \equiv \sigma \bmod 3$.

representations of O_3 by λ and κ from (6.2) so that $D^{0\lambda}(O_3)$ and $D^{1\lambda}(O_3)$ correspond to positive and negative representations (H p. 337) respectively. Restricting the operations of O_3 to $D^{[3,1]}(S_4)$, we have

$$D^{\kappa\lambda}(D^{[3,1]}(S_4)) = \sum_\alpha a_{\kappa\lambda\alpha} D^\alpha(S_4), \tag{6.3}$$

where the $a_{\kappa\lambda\alpha}$ are positive integers. Taking the characters for a class k of S_4, we have

$$\psi^{\kappa\lambda}(k) = \sum_\alpha a_{\kappa\lambda\alpha}\chi^\alpha(k), \tag{6.4}$$

$$a_{\kappa\lambda\alpha} = \sum_k \frac{g_k}{g}\, \psi^{\kappa\lambda}(k)(\chi^\alpha(k))^*, \tag{6.5}$$

which is the standard expression for the multiplicity a_α in terms of the characters of the groups involved. For the characters of O_3 with a rotation by an angle θ we have

$$\psi^{\kappa\lambda} = d^\kappa(q) \sum_{m=-\lambda}^{\lambda} \exp(im\theta), \qquad q = e, I, \qquad d^\kappa(e) = 1, \qquad d^\kappa(I) = (-1)^\kappa. \tag{6.6}$$

The particular rotation angles for the different classes of $S_4 \approx T_d$ are given by Jahn [22]) and reproduced in table 1. We decompose λ by writing $\lambda = 2\nu+\rho \equiv \rho \bmod 2$, $\rho = 0, 1$ and $\lambda \equiv \sigma \bmod 3$, $\sigma = 0, 1, 2$ and find the characters $\psi^{\kappa\lambda}(k)$ for the classes k of S_4 in terms of these numbers (table 1). All $\psi^{\kappa\lambda}$ are left unchanged on replacing λ by $\lambda' = \lambda+12$ except for class (1^4) where they are increased by 24. Since for this class $(g_k/g)(\chi^\alpha)^* = \frac{1}{24}$ we conclude, from (6.5), that $a_{\kappa\lambda'\alpha} = a_{\kappa\lambda\alpha}+1$ for all irreducible representations α of S_1.

From table 1 and (6.5) we obtain for the multiplicity of the representation [4] of S_4

$$a_{0\lambda[4]} = \tfrac{1}{24}(6(-1)^\nu+8(1-\sigma)+3(-1)^\rho+6(-1)^\rho+2\lambda+1), \tag{6.7}$$

which yields the first column of table 2. In a similar way the multiplicities given in table 2 are calculated up to $\lambda = 11$; as for higher values of λ we can use the relation

$$a_{\kappa\lambda\alpha} = a_{\kappa\beta\alpha}+\tau, \tag{6.8}$$

where $\lambda = 12\tau+\beta = \beta \bmod 12$, $\beta = 0, 1, \ldots, 11$.

TABLE 2

Multiplicity of irreducible representations $[\lambda]$ of $S_4 \approx T_d$ in a representation $D^{\kappa\lambda}(O_3)$

λ	κ	$[\lambda_1\lambda_2\lambda_3\lambda_4]$				
	0	[4]	[3,1]	[2,2]	[2,1²]	[1⁴]
	1	[1⁴]	[2,1²]	[2,2]	[3,1]	[4]
0		1	0	0	0	0
1		0	0	0	1	0
2		0	1	1	0	0
3		0	1	0	1	1
4		1	1	1	1	0
5		0	1	1	2	0
6		1	2	1	1	1
7		0	2	1	2	1
8		1	2	2	2	0
9		1	2	1	3	1
10		1	3	2	2	1
11		0	3	2	3	1

Compare ref. [29]).

(b) Next we look into the relation of Jacobi vectors (6.1) to fig. 1 and find that the transformations $D^{[3,1]}(S_4)$ correspond to the symmetry operations of the tetrahedron referred to the system $\dot{S} = (\dot{e}_1\dot{e}_2\dot{e}_3)$ of coordinates. We shall use rather the system $\ddot{S} = (\ddot{e}_1\ddot{e}_2\ddot{e}_3)$ which, in turn, corresponds to relative coordinates

$$\begin{aligned} \ddot{\eta}^1 &= \tfrac{1}{2}(\eta^1+\eta^3-\eta^2-\eta^4), \\ \ddot{\eta}^2 &= \tfrac{1}{2}(\eta^1+\eta^4-\eta^2-\eta^3), \\ \ddot{\eta}^3 &= \tfrac{1}{2}(\eta^1+\eta^2-\eta^3-\eta^4). \end{aligned} \tag{6.9}$$

Before we proceed we briefly state the notation for finite rotations as used in the book of Edmonds [28]) to which we refer as E. With a rotation matrix R, parametrized by angles $\alpha\beta\gamma$ denoting positive rotations around $\ddot{e}_3$-axis, new $\ddot{e}_2$-axis and new $\ddot{e}_3$-axis in that order,

$$R(\alpha\beta\gamma) = R(\gamma)R(\beta)R(\alpha), \tag{6.10}$$

we associate an operator $O(\alpha\beta\gamma)$ given by

$$O(\alpha\beta\gamma) = \mathrm{e}^{i\alpha\ddot{\Lambda}_3}\mathrm{e}^{i\beta\ddot{\Lambda}_2}\mathrm{e}^{i\gamma\ddot{\Lambda}_3}, \qquad \ddot{\Lambda}_t = \varepsilon_{rst}\ddot{\Lambda}^{rs}, \tag{6.11}$$

with the property

$$\begin{aligned} O(\alpha\beta\gamma)\langle\ddot{\eta}|\kappa\lambda\mu\rangle &= \langle R^{-1}\ddot{\eta}|\kappa\lambda\mu\rangle \\ &= \sum_{\mu'}\langle\ddot{\eta}|\kappa\lambda\mu'\rangle\langle\lambda\mu'|O(\alpha\beta\gamma)|\lambda\mu\rangle \\ &= \sum_{\mu'}\langle\ddot{\eta}|\kappa\lambda\mu'\rangle D^{\lambda}_{\mu'\mu}(\alpha\beta\gamma), \end{aligned} \tag{6.12}$$

where here, and in what follows, we shall use the notation

$$\langle\ddot{\eta}|\kappa\lambda\mu\rangle = \langle\ddot{\eta}|[h_1h_2h_3]\omega LM, \varphi\lambda\mu\rangle, \tag{6.13}$$

keeping only the quantum numbers κ (defined by (6.2)), λ and μ related to O_3 and its subgroups.

To each element of $S_4 \approx T_d$ corresponds a finite rotation $R(\alpha\beta\gamma)$ which for the elements of classes (21^2) and (4) is multiplied by an inversion I. For example, the transposition $(1, 2)$ corresponds to $(\ddot{e}_1\ddot{e}_2\ddot{e}_3) \to (-\ddot{e}_2-\ddot{e}_1\ddot{e}_3)$ and we denote it by $(\bar{2}\bar{1}3)$. We take out the inversion by writing $(\bar{2}\bar{1}3) = I(21\bar{3})$ and find for $(21\bar{3})$ the Euler angles $(0\ \pi\ \frac{1}{2}\pi)$, so that $I(0\ \pi\ \frac{1}{2}\pi)$ corresponds to the transposition $(1, 2)$. Table 3 gives all elements of $S_4 \approx T_d$ in this notation. The Euler angles take the values 0, $\frac{1}{2}\pi$, π, $\frac{3}{2}\pi$ and their effect on the states is given by the representation matrix

$$D^{\kappa\lambda}_{\mu'\mu}(\alpha\beta\gamma) = d^{\kappa}(q)\mathrm{e}^{i\mu'\alpha}d^{\lambda}_{\mu'\mu}(\beta)\mathrm{e}^{i\mu\gamma}, \qquad q = e, I. \tag{6.14}$$

We shall need the following properties of the $d^{\lambda}_{\mu'\mu}(\beta)$ (E p. 59):

$$d^{\lambda}_{\mu'\mu}(0) = \delta_{\mu'\mu}, \tag{6.15}$$

$$d^{\lambda}_{\mu'\mu}(\pi) = (-1)^{\lambda+\mu'}\delta_{\mu'-\mu}, \tag{6.16}$$

$$d^{\lambda}_{-\mu'\mu}(\tfrac{1}{2}\pi) = (-1)^{\lambda+\mu}d^{\lambda}_{\mu'\mu}(\tfrac{1}{2}\pi) = (-1)^{\mu+\mu'}d^{\lambda}_{\mu'-\mu}(\tfrac{1}{2}\pi). \tag{6.17}$$

(c) Instead of going from O_3 to S_4 directly, it proves more convenient to go first from O_3 to some subgroups of S_4 whose irreducible representations are easily obtained from those of O_3. The irreducible representations of these subgroups can be characterized by the eigenvalues of their SOC. The classification scheme derived in this way remains unaffected by the SOC of the full group S_4 since these operators commute with all SOC for subgroups of S_4.

TABLE 3

Transformation matrices $\bar{D}^{[3,1]}(\mathfrak{p})$ of the basis vectors $(\ddot{e}_1\ddot{e}_2\ddot{e}_3) = (123)$ of fig. 1 under the elements $\mathfrak{p}$ of S_4 in terms of Euler angles $(\alpha\beta\gamma)$ and inversions I

Class	Elements						
	$\mathfrak{p}$	e					
(1^4)	$\bar{D}(\mathfrak{p})$	(123)					
	I, (abc)	(000)					
	$\mathfrak{p}$	(1,2)	(1,3)	(1,4)	(2,3)	(2,4)	(3,4)
(21^2)	$\bar{D}(\mathfrak{p})$	$(\bar{2}\bar{1}3)$	$(1\bar{3}\bar{2})$	$(\bar{3}2\bar{1})$	(321)	(132)	(213)
	I, (abc)	I(021)	I(111)	I(012)	I(210)	I(313)	I(023)
	$\mathfrak{p}$	(1,2)(3,4)	(1,3)(2,4)	(1,4)(2,3)			
(2^2)	$\bar{D}(\mathfrak{p})$	$(\bar{1}\bar{2}3)$	$(1\bar{2}\bar{3})$	$(\bar{1}2\bar{3})$			
	I, (abc)	(200)	(220)	(020)			
	$\mathfrak{p}$	(1,2,3)	(1,3,2)	(1,2,4)	(1,4,2)	(1,3,4)	(1,4,3)
(31)	$\bar{D}(\mathfrak{p})$	$(3\bar{1}\bar{2})$	$(\bar{2}\bar{3}1)$	$(\bar{2}3\bar{1})$	$(\bar{3}\bar{1}2)$	$(\bar{3}1\bar{2})$	$(2\bar{3}\bar{1})$
	I, (abc)	(312)	(013)	(211)	(110)	(310)	(213)
	$\mathfrak{p}$	(2,3,4)	(2,4,3)				
	$\bar{D}(\mathfrak{p})$	(231)	(312)				
	I, (abc)	(011)	(112)				
	$\mathfrak{p}$	(1,2,3,4)	(2,1,4,3)	(1,2,4,3)	(2,1,3,4)	(1,3,2,4)	(4,2,3,1)
(4)	$\bar{D}(\mathfrak{p})$	$(\bar{1}3\bar{2})$	$(\bar{1}\bar{3}2)$	$(3\bar{2}\bar{1})$	$(\bar{3}\bar{2}1)$	$(\bar{2}1\bar{3})$	$(2\bar{1}\bar{3})$
	I, (abc)	I(113)	I(311)	I(010)	I(212)	I(100)	I(300)

$(\alpha\beta\gamma)$ are given by (abc) where $\alpha = a\frac{1}{2}\pi$, $\beta = b\frac{1}{2}\pi$, $\gamma = c\frac{1}{2}\pi$.

The group $S_4 \approx T_d$ has D_{2d} as the largest subgroup which leaves invariant the $\ddot{e}_3$ axis up to a reflection. The elements and classes are given in table 4, the characters of D_{2d} are given in H p. 126. In order to diagonalize the SOC we introduce the real spherical harmonics [31])

$$\langle \ddot{\eta}|\kappa\lambda|\mu|\rho\rangle = (i)^{\frac{1}{2}(\rho-1)+\mu} g_\mu [\langle \ddot{\eta}|\kappa\lambda|\mu|\rangle + \rho(-1)^\lambda \langle \ddot{\eta}|\kappa\lambda - |\mu|\rangle],$$
$$g_\mu = \sqrt{\frac{1}{2(1+\delta_{\mu 0})}}, \tag{6.18}$$

with $\rho = \pm 1$ which are real for the phase condition (E p. 21)

$$|\lambda\mu\rangle^* = (-1)^{\lambda+\mu}|\lambda-\mu\rangle.$$

These combinations correspond to a subgroup which may be denoted as $D_\infty \times \mathfrak{J} \subset O_3$, where D_∞ consists of all rotations in the $(\ddot{e}_1, \ddot{e}_2)$-plane and of the element (1, 4)(2, 3) corresponding to a rotation by π around the $\ddot{e}_2$-axis. The states (6.18) are characterized by ρ and by the eigenvalue $|\mu|^2$ of $(\ddot{A}_3)^2$. Moreover, they are eigenstates of the SOC of D_{2d} with eigenvalues given in table 4 where

TABLE 4

Group D_{2d}

Class k	Elements	Eigenvalue of $\mathfrak{K}^{(k)}$
E	e	1
$C_2{}^a$	(1,2)(3,4)	$2\varepsilon^2-1$
S_4	(1,3,2,4), (4,2,3,1)	$2\varepsilon(-1)^\kappa$
$C_2{}^b$	(1,3)(2,4), (1,4)(2,3)	$2\rho\varepsilon^2$
σ_d	(1,2), (3,4)	$2\rho\varepsilon(-1)^\kappa$

The symbols κ, ρ and ε are defined in (6.2), (6.18), (6.19), respectively.

$$\varepsilon = \tfrac{1}{2}(i^{|\mu|} + i^{-|\mu|}), \tag{6.19}$$

so that it takes the values $\varepsilon = 1, 0, -1$ for $|\mu| \equiv 0 \bmod 4$, $|\mu| \equiv 1$ or $3 \bmod 4$, $|\mu| \equiv 2 \bmod 4$, respectively. It is advantageous to add ε to the quantum numbers κ, λ, $|\mu|$, ρ though from (6.19) it is clearly not independent of $|\mu|$. The reason for keeping it is that the states we are interested in are in the chain $O_3 \supset T_d \supset D_{2d}$ which is different from the chain $O_3 \supset D_\infty \times \mathfrak{J} \supset D_{2d}$ so that $(\ddot{A}_3)^2$ in general is not diagonal. In contrast to this the classification in terms of ρ and ε is significant for both chains. We therefore denote the states in the chain $O_3 \supset D_\infty \times \mathfrak{J} \supset D_{2d}$ by

$$\langle \ddot{\eta}|\kappa\lambda|\mu|\rho\varepsilon\rangle. \tag{6.20}$$

(d) We found that the representations of S_4 in general are repeated in a given representation of O_3. How can we distinguish between them? A similar problem was solved for the chain of groups $\mathscr{U}_3 \supset \mathscr{R}_3$ by introducing the operator Ω in BM II. We state some general properties of Ω: (i) Ω is constructed from the generators of $\mathscr{U}_3$ and therefore commutes with all invariant operators defining the representation of $\mathscr{U}_3$, (ii) Ω is a scalar under R_3 and therefore commutes with all generators of $\mathscr{R}_3$ while it is not a function only of them, (iii) no eigenvalue of Ω is repeated for a given representation of $\mathscr{R}_3$ so that this operator solves the multiplicity problem. We generalize these conditions to the chain $O_3 \supset T_d \approx S_4$ and ask for an operator X with the properties that (i) X is constructed from the generators $\ddot{\Lambda}_1, \ddot{\Lambda}_2, \ddot{\Lambda}_3$ or R_3 and therefore, commutes with $\ddot{\Lambda}^2$, (ii) X is invariant under all permutations of S_4, (iii) no eigenvalue χ of X is repeated for a given representation of S_4.

In order to find an operator with these properties, we notice from the general analysis in sect. 3, that $\ddot{\Lambda}_1, \ddot{\Lambda}_2, \ddot{\Lambda}_3$ transform under O_3 according to the representation $D^{01}(O_3)$, i.e. like a pseudovector, and under S_4 according to the representation $D^{[2,1^2]}(S_4)$. If we now couple $\ddot{\Lambda}_1, \ddot{\Lambda}_2, \ddot{\Lambda}_3$ with Clebsch-Gordan coefficients of R_3 to Racah tensors u^t_τ, $\tau = t, \ldots, -t$, they will transform under O_3 according to the representation $D^{0t}(O_3)$. For these representations we find from table 2, that representations $D^{[4]}(S_4)$ are contained in $D^{00}, D^{04}, D^{06}, \ldots$. The Racah tensor u^0 corresponds to Λ^2. Therefore the lowest operator $X(\ddot{\Lambda}_1\ddot{\Lambda}_2\ddot{\Lambda}_3)$ independent of Λ^2 and invariant under permutations, is a linear combination of Racah tensors u^4_τ, $\tau = 4, \ldots, -4$. From the work of Jahn [29] we find that the required operator with symmetry [4] under S_4 is given by

$$X = \tfrac{1}{2}\sqrt{\tfrac{5}{6}}(u^4_4+u^4_{-4})+\tfrac{1}{2}\sqrt{\tfrac{7}{3}}u^4_0. \tag{6.21}$$

In cartesian coordinates, X is given essentially by $(\ddot{\Lambda}_1)^4+(\ddot{\Lambda}_2)^4+(\ddot{\Lambda}_3)^4$. Certainly X has the properties 1 and 2, and we shall show that it also has the property 3. For this we shall use the matrix elements of X.

The Racah tensors u^t formed from the $\ddot{\Lambda}_s$ clearly commute with Λ^2 and therefore their matrix elements are diagonal in λ. Choosing the normalization coefficient in such a way that the reduced matrix element becomes

$$\langle\lambda||u^t||\lambda\rangle = (2t+1)^{\frac{1}{2}}, \tag{6.22}$$

we could write the matrix elements in terms of Clebsch-Gordan coefficients, i.e. (E p. 75)

$$\langle\lambda\mu'|u^t_\tau|\lambda\mu\rangle = (-1)^{\lambda-\mu}(\lambda\mu'\lambda-\mu|t\tau). \tag{6.23}$$

Therefore we find the matrix elements of X

$$\langle\kappa'\lambda'\mu'|X|\kappa\lambda\mu\rangle = \tfrac{1}{2}\delta_{\kappa'\kappa}(-1)^{\lambda-\mu} \times\left[\sqrt{\tfrac{5}{6}}\left((\lambda\mu'\lambda-\mu|44)+(\lambda\mu'\lambda-\mu|4-4)\right)+\sqrt{\tfrac{7}{3}}(\lambda\mu'\lambda-\mu|40)\right], \tag{6.24}$$

with symmetries

$$\langle\kappa\lambda\mu'|X|\kappa\lambda\mu\rangle = \langle\kappa\lambda\mu|X|\kappa\lambda\mu'\rangle = \langle\kappa\lambda-\mu'|X|\kappa\lambda-\mu\rangle.$$

From these symmetries and (6.24) we find in the chain

$$
\begin{aligned}
& O_3 \supset D_\infty \times \mathfrak{I} \supset D_{2d}: \\
& \langle \kappa\lambda\rho'\mu'\varepsilon'|X|\kappa\lambda\rho\mu\varepsilon\rangle \\
& = \tfrac{1}{2} g_{\mu'\mu}\delta_{\rho'\rho}(-1)^{\lambda-\mu}[\sqrt{\tfrac{5}{6}}\{(\lambda\mu'\lambda-\mu|44)+\rho(-1)^{\lambda}(\lambda\mu'\lambda\mu|44)\} \\
& +\sqrt{\tfrac{7}{3}}\{(\lambda\mu'\lambda-\mu|40)+\rho(-1)^{\lambda}(\lambda\mu'\lambda\mu|40)\}],
\end{aligned} \tag{6.25}
$$

where

$$g_{\mu'\mu} = 2g_{\mu'}g_{\mu}, \qquad \mu' = |\mu'| \geqq 0, \qquad \mu = |\mu| \geqq 0.$$

We conclude that X does not mix states with different ρ. In addition we find for all matrix elements $\varepsilon'(\mu') = \varepsilon(\mu)$. Both properties are to be expected since X commutes with all permutation of S_4 and therefore cannot mix states defined by eigenvalues of SOC from the algebra $\mathfrak{A}$ of S_4. The matrix of X splits, therefore, into six submatrices which we denote by $\boldsymbol{\beta}^{\rho\varepsilon}$. For each submatrix we can show, by a reasoning completely analogous to that applied in BM II to the matrix of Ω, that it has no repeated eigenvalue. To do this we notice from (6.25) that the off-diagonal matrix elements of X contain the Clebsch-Gordan coefficient (E p. 44)

$$
\begin{aligned}
(\lambda\mu'\lambda-\mu|44) = {} & \Delta(\lambda,\lambda,4)\delta_{\mu'-\mu,4} \\
& \times(-1)^{\lambda-\mu}\left[\frac{9!(2\lambda-4)!(\lambda+\mu+4)!(\lambda-\mu)!}{(4!)^2(2\lambda+5)!(\lambda-\mu-4)!(\lambda+\mu)!}\right]^{\frac{1}{2}},
\end{aligned} \tag{6.26}
$$

where $\Delta(\lambda,\lambda,4)$ denotes the triangle condition. Clearly (6.26) is different from zero for $\lambda \geqq 2$ provided $\mu'-\mu = 4$. But the cases $\lambda = 0, 1$ offer no multiplicity problem so that in all cases of multiplicity the off-diagonal matrix elements of X are different from zero. From this and the shape of the matrix $\boldsymbol{\beta}^{\rho\varepsilon}$ for $\varepsilon = \pm 1$ it follows that its properties are identical to those of the corresponding matrix $\boldsymbol{\beta} = (\beta_{qq'})$ appearing in BM II. We conclude therefore that for $\varepsilon = \pm 1$ no eigenvalue is repeated. For the submatrices $\boldsymbol{\beta}^{\rho 0}$ we have a slightly different shape which does, however, not change the essence of the reasoning used in BM II, so that there are no repeated eigenvalues for $\varepsilon = 0$ (appendix 2).

We cannot, by this reasoning, prove that the eigenvalues χ of X are different for different submatrices $\boldsymbol{\beta}^{\rho\varepsilon}$, and this is, in fact, not true. If we denote the matrix elements of $\boldsymbol{\beta}^{\rho 0}$ by $(\beta^{\rho 0}_{ik})$, where $|\mu'| = 2i+1$, $|\mu| = 2k+1$ and define a matrix $\boldsymbol{A}$ with elements $a_{ik} = (-1)^{i+1}\delta_{ik}$, we obtain the equivalence

$$\boldsymbol{\beta}^{-10} = \boldsymbol{A}\boldsymbol{\beta}^{10}\boldsymbol{A}^{-1}, \tag{6.27}$$

which shows that all eigenvalues of $\boldsymbol{\beta}^{10}$ are repeated in $\boldsymbol{\beta}^{-10}$ (appendix 2). From the properties of X, a certain repetition of eigenvalues is to be expected since X should distinguish between different representations of S_4 whereas it should be degenerate with respect to the subgroups of S_4 which label the rows of the representation, in a similar way as Ω is degenerate with respect to the representations of $\mathscr{R}_2$ in $\mathscr{U}_3 \supset \mathscr{R}_3 \supset \mathscr{R}_2$.

Therefore we obtain a complete characterization of the states in the chain $O_3 \supset T_d \approx S_4 \supset D_{2d}$ by adding to χ the quantum numbers ρ and ε writing

$$\langle \ddot{\boldsymbol{\eta}} | \kappa\lambda\chi\rho\varepsilon \rangle = \langle \ddot{\boldsymbol{\eta}} | [h_1 h_2 h_3]\omega LM, \varphi\lambda\chi\rho\varepsilon \rangle. \tag{6.28}$$

(e) The fact that the repeated eigenvalues of X belong to different submatrices $\boldsymbol{\beta}^{\rho\varepsilon}$ proves that the basis functions of a given irreducible representation of $S_4 \approx T_d$ may be distinguished by ρ, ε corresponding to the chain $T_d \supset D_{2d}$. In order to find the significance of these numbers with respect to representations of S_4 derived from the canonical chain $S_4 \supset S_3 \supset S_2 \supset S_1$, we should now apply the corresponding projection operators to the states (6.28). It suffices, however, to apply them to the states (6.20) in the chain $O_3 \supset D_\infty \times \mathfrak{F} \supset D_{2d}$ since the numbers ρ, ε correspond to the group D_{2d} which is a member of both chains.

First we form the SOC (3.6) for the classes with cycle structure (1^4), $(2\ 1^2)$, (2^2), $(3\ 1)$, (4) of S_4 and take their matrix elements between the states (6.20) which are diagonal in ρ, ε for the reasons mentioned in (c). These matrix elements are given by

$$\begin{aligned}
\langle \kappa\lambda\mu'\rho\varepsilon | \mathfrak{K}^{(1^4)} | \kappa\lambda\mu\rho\varepsilon \rangle &= \delta_{\mu'\mu}, \\
\langle \kappa\lambda\mu'\rho\varepsilon | \mathfrak{K}^{(21^2)} | \kappa\lambda\mu\rho\varepsilon \rangle &= (-1)^\kappa [2\rho\varepsilon\delta_{\mu'\mu} + 4(2\varepsilon^2 + \rho - 1) g_{\mu'\mu} d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi)], \\
\langle \kappa\lambda\mu'\rho\varepsilon | \mathfrak{K}^{(31)} | \kappa\lambda\mu\rho\varepsilon \rangle &= 8\varepsilon(1+\rho) g_{\mu'\mu} d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi), \\
\langle \kappa\lambda\mu'\rho\varepsilon | \mathfrak{K}^{(2^2)} | \kappa\lambda\mu\rho\varepsilon \rangle &= [2\varepsilon^2(\rho+1) - 1]\delta_{\mu'\mu}, \\
\langle \kappa\lambda\mu'\rho\varepsilon | \mathfrak{K}^{(4)} | \kappa\lambda\mu\rho\varepsilon \rangle &= (-1)^\kappa [2\varepsilon\delta_{\mu'\mu} + 4\{1 + \rho(2\varepsilon^2 - 1)\} g_{\mu'\mu} d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi)], \\
\mu' = |\mu'|, \qquad \mu &= |\mu|.
\end{aligned} \tag{6.29}$$

From the SOC we build the projection operators (3.10) with the characters of S_4 given in table 1 and find, for example,

$$\langle \kappa\lambda\mu'\rho\varepsilon | \mathfrak{P}^{[4]} | \kappa\lambda\mu\rho\varepsilon \rangle = \tfrac{1}{12}\varepsilon^2(1+\rho)[1 + \varepsilon(-1)^\kappa][\delta_{\mu'\mu} + (-1)^\kappa g_{\mu'\mu} d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi)], \tag{6.30}$$

so that we have non-vanishing contributions to irreducible representations $D^{[4]}(S_4)$ for $\kappa = 0$, $\rho = +1$, $\varepsilon = +1$ and for $\kappa = 1$, $\rho = +1$, $\varepsilon = -1$. Using the projection operators for the different irreducible representations of S_4 we obtain the assignment of table 5 in terms of κ, ρ, ε. We notice that for all projection operators replacing $\kappa = 0$ by $\kappa = 1$ is equivalent to replacing the characters of classes $(2\ 1^2)$ and (4) by their negatives so that the associated partitions are obtained.

Now we identify the different basis functions for the two and three dimensional representations. The simple transformation properties of the vectors $\ddot{\boldsymbol{\eta}}^s$ under T_d and D_{2d} suggest that in the $[3, 1]$ representation we first should look for combinations transforming like $\ddot{\boldsymbol{\eta}}^1$, $\ddot{\boldsymbol{\eta}}^2$, $\ddot{\boldsymbol{\eta}}^3$ and return then to the Yamanouchi representation by a linear transformation.

Table 3 gives the representation $\bar{D}^{[3,1]}(S_4)$ spanned by $\ddot{\boldsymbol{\eta}}^1$, $\ddot{\boldsymbol{\eta}}^2$, $\ddot{\boldsymbol{\eta}}^3$. To find a basis function belonging to this representation, we employ Wigner projection operators (ref. [14]), p. 117)

$$\mathfrak{P}_{jj}^{[3,1]} = \frac{n_{[3,1]}}{4!} \sum_{\mathfrak{p}\in S_4} (\bar{D}_{jj}^{[3,1]}(\mathfrak{p}))^* \cdot \mathfrak{p} \tag{6.31}$$

given in terms of the representation matrices $\bar{D}^{[3,1]}$, whose elements we denote by numbers 1, 2, 3 corresponding to $\ddot{\eta}^1, \ddot{\eta}^2, \ddot{\eta}^3$. By applying $\mathfrak{P}_{33}^{[3,1]}$ we obtain non-vanishing results only if $\varepsilon(-1)^x = -1$, in which cases

$$\langle\kappa\lambda\rho'\mu'\varepsilon'|\mathfrak{P}_{33}^{[3,1]}|\kappa\lambda\rho\mu\varepsilon\rangle = \delta_{\rho'\rho}\delta_{\mu'\mu}\delta_{\varepsilon'\varepsilon}. \tag{6.32}$$

We denote these basis functions by $[3, 1]_3$. In a similar way we find $[3, 1]_2$ and $[3, 1]_1$ in terms of κ, ρ, ε. On replacing the vector components $\ddot{\eta}^1, \ddot{\eta}^2, \ddot{\eta}^3$ by those of a pseudo-vector with respect to O_3 we obtain a basis for the $[2, 1^2]$ representation. This representation differs from $\bar{D}^{[3,1]}(S_4)$ only by a minus sign for all odd permutations. By means of projection operators similar to (6.31) we find the basis functions $[2, 1^2]_s$

TABLE 5

Relations between the states characterized by the irreducible representations of $S_4 \approx T_d$ and the states characterized by κ, ρ, ε

		$\rho = +1$	$\rho = -1$
$\kappa = 0$	$\varepsilon = +1$	$[2,2]_2$, $[4]$	$[2,1^2]_3$
	$\varepsilon = -1$	$[2,2]_1$, $[1^4]$	$[3,1]_3$
	$\varepsilon = 0$	$[3,1]_1$, $[2,1^2]_1$	$[3,1]_2$, $[2,1^2]_2$
$\kappa = 1$	$\varepsilon = +1$	$[2,2]_1$, $[1^4]$	$[3,1]_3$
	$\varepsilon = -1$	$[2,2]_2$, $[4]$	$[2,1^2]_3$
	$\varepsilon = 0$	$[2,1^2]_1$, $[3,1]_1$	$[2,1^2]_2$, $[3,1]_2$

The set κ, ρ, ε defines the representation of the subgroup D_{2d} of T_d according to table 4. The lower indices of the partitions refer to the rows of the representation of T_d.

with $s = 1, 2, 3$ and give them in terms of κ, ρ, ε in table 5 together with the $[3,1]_s$. The basis functions $[3, 1]_s$ and $[2, 1]_s$ with $s = 1, 2$ can be obtained including phases by the application of the transpositions (1, 3) and (1, 4) respectively to $[3, 1]_3$ and $[2, 1^2]_3$ basis functions (appendix 3).

Now we return to the Yamanouchi representation by noting that

$$\begin{pmatrix} \dot{\eta}^1 \\ \dot{\eta}^2 \\ \dot{\eta}^3 \end{pmatrix} = \mathfrak{M} \begin{pmatrix} \ddot{\eta}^1 \\ \ddot{\eta}^2 \\ \ddot{\eta}^2 \end{pmatrix}, \qquad \mathfrak{M} = \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 \\ -\sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{2}{3}} \\ \sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} \end{pmatrix}. \tag{6.33}$$

Consequently the basis functions with Yamanouchi symbols are given by

$$[3, 1]: \begin{pmatrix} \phi(1121) \\ \phi(1211) \\ \phi(2111) \end{pmatrix} = \mathfrak{M} \begin{pmatrix} [3, 1]_1 \\ [3, 1]_2 \\ [3, 1]_3 \end{pmatrix}, \tag{6.34}$$

$$[2, 1^2]: \begin{pmatrix} \phi(1321) \\ \phi(3121) \\ \phi(3211) \end{pmatrix} = \mathfrak{M} \begin{pmatrix} [2,1^2]_1 \\ [2, 1^2]_2 \\ [2, 1^2]_3 \end{pmatrix}. \tag{6.35}$$

Next we consider the [2, 2] representation which from table 5 has $\kappa = 0, 1$, $\rho = 1$, $\varepsilon = \pm 1$. We apply to these states the transposition (1, 2) and find from this the states with Yamanouchi symbols

$$\begin{aligned} \phi(2211) &= [2, 2]_2, \qquad \varepsilon(-1)^\kappa = 1, \\ \phi(2121) &= [2, 2]_1, \qquad \varepsilon(-1)^\kappa = -1. \end{aligned} \tag{6.36}$$

(f) The assignments of table 5 remain valid for the states (6.28) with the advantage that for them the multiplicity problem is solved completely. In particular cases like for the repeated basis functions $[3,1]_3$ and $[2,1^2]_3$ we may replace X by the simpler operator $(\ddot{\Lambda}_3)^2$ with eigenvalue $|\mu|^2$ as was done in ref. [29]). In general, the repeated eigenvalues χ together with their values of κ, ρ, ε determine the basis of the representations [3, 1], [2, 1^2] and [2, 2]. If by accident the eigenvalues χ, χ' of a representation [4] with $\varepsilon = (-1)^\kappa$ and a representation [1^4] with $\varepsilon = -(-1)^\kappa$ coincide, we distinguish between them by projection operators like (6.30). In the next step we replace the numbers κ, ρ, ε by Yamanouchi symbols using the relations (6.33–6.35).

We return now to the Jacobi vectors $\dot{\boldsymbol{\eta}}^s$ and do this by writing $\mathfrak{M}$ from (6.33) as a rotation matrix

$$\mathfrak{M} = R(\gamma_0)R(\beta_0)R(\alpha_0), \tag{6.37}$$

finding $\alpha_0 = \frac{1}{2}\pi$, $\cos\beta_0 = \sqrt{\frac{1}{3}}$, $\sin\beta_0 = \sqrt{\frac{2}{3}}$, $\gamma_0 = -\frac{1}{4}\pi$. Consequently we have

$$\langle \ddot{\boldsymbol{\eta}}|\kappa\lambda\mu\rangle = \sum_{\mu'} \langle \dot{\boldsymbol{\eta}}|\kappa\lambda\mu'\rangle D^{\lambda}_{\mu'\mu}(\alpha_0\beta_0\gamma_0), \tag{6.38}$$

which we may rewrite in terms of the states (6.20) by means of (6.18).

In which way could we then construct states of four particles with permutational symmetry? First we would take out the centre-of-mass motion and consider the chain $U_{12} \supset \mathscr{U}_3 \times U_4$, $U_4 \supset U_3$. We would use the vectors $\ddot{\boldsymbol{\eta}}^s$ from (6.9) and obtain the states of highest weight in $\mathscr{U}_3$ in the chain $U_3 \supset R_3 \supset R_2$ by applying $\ddot{\Lambda}_-$ to a polynomial similar to the one given in BM II for the chain $\mathscr{U}_3 \supset \mathscr{R}_3 \supset \mathscr{R}_2$. We could also make ϕ (corresponding to Ω in BM II) diagonal for these states. Next we transform to the chain $U_3 \supset O_3 \supset D_\infty \times \mathfrak{F} \supset D_{2d}$ by means of (6.18). By diagonalizing X we obtain the states (6.28). For these states, table 5 together with the relations (6.33–6.35) gives the combinations with definite Yamanouchi symbol. Finally we return to Jacobi vectors by means of the rotation (6.38) and apply lowering operators in $\mathscr{U}_3$ to get states in the $\mathscr{U}_3 \supset \mathscr{U}_2 \supset \mathscr{U}_1$ chain, from which we transform [7]) to the $\mathscr{U}_3 \supset \mathscr{R}_3 \supset \mathscr{R}_2$ chain. Our states are then characterized by

$$\langle \ddot{\boldsymbol{\eta}}|\,[h_1h_2h_3]\omega LM,\, \varphi\lambda\chi(r_4r_3r_2r_1)\rangle. \tag{6.39}$$

7. Construction of n-Particle States with Permutational Symmetry

The analysis of the four-particle states given in sect. 6 together with the results of sects. 2–4, enable us to outline a general procedure for obtaining n-particle states with permutational symmetry in a harmonic oscillator.

We would first take out the centre-of-mass motion for this n-particle system which implies that we express our states in terms of Jacobi vectors $\dot{\boldsymbol{\eta}}^s$, $s = 1, 2, \ldots n-1$ acting on the ground state $|0\rangle$, allowing no excitation in $\dot{\boldsymbol{\eta}}^n$, i.e., we consider directly the $\mathscr{U}_3 \times U_{n-1}$ subgroup of U_{3n}.

We then obtain explicitly the state of highest weight both in $\mathscr{U}_3$ and in the subgroup $O_{n-1} \supset R_{n-1}$ of U_{n-1}. This implies that we look for polynomials that satisfy both

$$\mathscr{C}_{ij}P = 0, \qquad i < j \qquad i, j = 1, 2, 3, \qquad \mathscr{C}_{ii}P = h_i P, \qquad i = 1, 2, 3, \tag{7.1}$$

and equations involving the generators $\dot{\Lambda}^{st}$ of R_{n-1}, of the type discussed in eq. (5.20) of ref. [32]). These polynomials correspond to an irreducible representation of R_{n-1} characterized by, at most, three partition numbers† $(\lambda_1 \lambda_2 \lambda_3)$ since U_{n-1} in turn has only three partion numbers $(h_1 h_2 h_3)$ for our states. The polynomials have been explicitly derived by Chacón [33]) and will be discussed elsewhere. The polynomials are not completely defined by the above equations and need, for their full characterization, a set of commuting operators which are of the same type as the Ω in the $\mathscr{U}_3 \supset \mathscr{R}_3$ chain. It is possible to show [33]) that in our case one needs no more than three operators ϕ_1, ϕ_2, ϕ_3 to define completely the most general state of highest weight in R_{n-1}.

From the state of highest weight in both $\mathscr{U}_3$ and R_{n-1} we obtain a complete set of states by using the lowering operators for both the $\mathscr{U}_3 \supset \mathscr{U}_2 \supset \mathscr{U}_1$ chain (the operators $\mathscr{L}_{ki}$ of sect. 2) and the $R_{n-1} \supset R_{n-2} \supset \ldots \supset R_2$ chain. Particular cases of the latter operators have been derived in recent publications [34]) and a systematic discussion of their explicit form and properties has been given by Nagel and Pang [35]). The passage from the $\mathscr{U}_3 \supset \mathscr{U}_2 \supset \mathscr{U}_1$ chain to the $\mathscr{U}_3 \supset \mathscr{R}_3 \supset \mathscr{R}_2$ chain can be achieved either with the transformation brackets of ref. [7]) or with the eigenvectors associated with the matrix of L^2 with respect to the states decribed by the $\mathscr{U}_3 \supset \mathscr{U}_2 \supset \mathscr{U}_1$ chain [36]).

All the steps necessary for the derivation of the states characterized by the chains of subgroups

$$U_{3n} \supset \mathscr{U}_3 \times U_n, \tag{7.2a}$$

$$\mathscr{U}_3 \supset \mathscr{R}_3 \supset \mathscr{R}_2, \qquad U_n \supset U_{n-1} \supset O_{n-1}, \tag{7.2b, c}$$

$$O_{n-1} \supset R_{n-1} \supset R_{n-2} \supset \ldots \supset R_2 \tag{7.2d}$$

are then available, but this is not yet the chain that gives states with permutational symmetry.

From the discussion of the four-particle problem in the previous section we see that rather than the chain (7.2d), we require the reduction of the representations of O_{n-1}

† The same symbols λ are used for the irreducible representations of O_{n-1} as for S_n, but no confusion arises because of the different number of subindices as well as the context in which they appear.

in the chain

$$O_{n-1} \supset D^{[n-1,1]}(S_n). \tag{7.2e}$$

This requires a set of commuting operators $X_1, X_2, \ldots$ invariant under S_n and formed from the generators $\dot{A}^{st}$ of O_{n-1} which will play, in chain (7.2e), the same role as X plays for the $O_3 \supset D^{[3,1]}(S_4)$ chain. The matrix elements of the operators X_i with respect to states characterized by the chain $R_{n-1} \supset \ldots \supset R_2$ can readily be obtained from the matrix elements of the generators $\dot{A}^{st}$ with respect to states characterized by the same chain which have been derived by Gelfand and Zetlin [37]). From the eigenvectors associated with these matrices one could obtain the states in the chain $O_{n-1} \supset D^{[n-1,1]}(S_4)$ from those in the chain $O_{n-1} \supset R_{n-1} \supset \ldots \supset R_2$. Finally, with the help of the projection operators in the chain $S_n \supset S_{n-1} \supset \ldots \supset S_1$ one would get states completely defined by the eigenvalues $\chi_1, \chi_2 \ldots$ of the X_i and by the Yamanouchi symbols, i.e.

$$\langle \dot{\eta} | [h_1 h_2 h_3] \omega LM, \varphi_1 \varphi_2 \varphi_3 (\lambda_1 \lambda_2 \lambda_3) \chi_1 \chi_2 \ldots (r_n r_{n-1} \ldots r_1) \rangle. \tag{7.3}$$

While the procedure for deriving the states (7.3) is straightforward, it is in general quite laborous. Particular cases of considerable physical importance, such as when $h_1 \neq 0$, $h_2 = h_3 = 0$, can be solved much more simply and they will be discussed in detail when we analyse some problems connected with clustering in other papers of this series.

Appendix 1

PERMUTATIONAL SYMMETRY OF THE GENERATORS OF U_{n-1}

We look for linear combinations of the generators $\dot{C}^{st}$, $1 \leqq s, t \leqq n-1$ of U_{n-1} with permutational symmetry corresponding to definite Yamanouchi symbols and first consider the irreducible representation $[n-1, 1]$ of S_n. A combination with Yamanouchi symbol $Y = (21^{n-1})$ should fulfill

$$(i, k)\dot{C}(21^{n-1}) = \dot{C}(21^{n-1}), \qquad i < k \leqq n-1 \tag{A.1}$$

and from the discussion in sect. 3 should be symmetric with respect to the indices s, t and traceless. These conditions lead to

$$\dot{C}(21^{n-1}) = \sqrt{\frac{1}{(n-1)(n-2)}} \left(\sum_{s=1}^{n-2} \dot{C}^{ss} - (n-2)\dot{C}^{n-1\, n-1}\right),$$

which gives, on applying the ladder procedure (3.4), the rèsult (3.23).

For the representation $[n-2, 2]$ we first consider $\dot{C}(221^{n-2})$ which should fulfill

$$(i, k)\dot{C}(221^{n-2}) = \dot{C}(221^{n-2}), \qquad i < k \leqq n-2, \tag{A.2}$$

$$(n-1, n)\dot{C}(221^{n-2}) = \dot{C}(221^{n-2}) \tag{A.3}$$

and should again be traceless and symmetric. A solution is given by

$$\dot{C}(221^{n-2}) = \frac{1}{n-2}\sqrt{\frac{1}{(n-1)(n-3)}}\Big[\sum_{s=1}^{n-3}\dot{C}^{ss}-(n-3)\dot{C}^{n-2\,n-2} -\tfrac{1}{2}(n-3)\sqrt{n(n-2)}(\dot{C}^{n-1\,n-2}+\dot{C}^{n-2\,n-1})\Big] \quad (3.24)$$

and is unique up to additional terms containing $\dot{C}^{n-1n-1}$. The ladder procedure applied to (3.24) gives (3.25). From (3.25) one obtains $\dot{C}(1^{n-4}2121)$ with the property

$$(1,2)\dot{C}(1^{n-4}2121) = \dot{C}(1^{n-4}2121). \quad (A.4)$$

Since an additional term proportional to $\dot{C}^{n-1n-1}$ would result in similar terms for all functions derived by the ladder procedure, the condition (A.4) would not hold. Therefore (3.24) is the correct ansatz.

Appendix 2

NON-DEGENERACY OF X

We want to show that the matrices $\beta^{\rho\varepsilon}$ of X defined in sect. 6(d) have no degenerate eigenvalue. This is obvious for $\varepsilon = \pm 1$ since the properties of these matrices allow for the same reasoning as the matrix of the operator Ω discussed in BM II. For $\varepsilon = 0$, $|\mu'|$ and $|\mu|$ are odd and we introduce new indices $|\mu| = 2k+1$, $|\mu'| = 2i+1$, $k, i = 0, 1, 2, \ldots j$. The eigenvalue equation of the matrix $\boldsymbol{\beta}^{\rho 0} = (\beta_{ik})$ from (6.25) is given by

$$\begin{aligned}
&\beta_{00}a_0+\beta_{01}a_1+\beta_{02}a_2 &&= \chi a_0,\\
&\beta_{10}a_0+\beta_{11}a_1+\beta_{13}a_3 &&= \chi a_1,\\
&\beta_{20}a_0+\beta_{22}a_2+\beta_{24}a_4 &&= \chi a_2,\\
&\quad\vdots \qquad\quad \vdots \qquad\quad \vdots && \quad\vdots\\
&\beta_{j-2j-4}a_{j-4}+\beta_{j-2j-2}a_{j-2}+\beta_{j-2j}a_j &&= \chi a_{j-2},\\
&\beta_{j-1j-3}a_{j-3}+\beta_{j-1j-1}a_{j-1} &&= \chi a_{j-1},\\
&\beta_{jj-2}a_{j-2}+\beta_{jj}a_j &&= \chi a_j,
\end{aligned} \quad (A.5)$$

where for $i \neq k$ $\beta_{ik} \neq 0$ according to (6.26). Assuming j even we obtain, when $a_j = 0$, starting from the last row of (A.5), $0 = a_{j-2} = a_{j-4} = \ldots = a_0$. From rows $1, 2, 4, 6 \ldots j-1$ we find then $0 = a_1 = a_3 = \ldots = a_{j-1}$. If j is odd, we find when $a_j = 0$ that $0 = a_{j-2} = a_{j-4} \ldots = a_1$ and from rows $2, 1, 3, 5 \ldots j-1 : 0 = a_0 = a_2 = \ldots = a_{j-1}$. Therefore if $a_j = 0$, all coefficients a_i are equal to zero. But from this property of the matrices $\boldsymbol{\beta}^{\rho 0}$ it follows, as was shown in BM II, that all eigenvalues are non-degenerate.

From (6.25) it can be seen that the matrices $\boldsymbol{\beta}^{10}$ and $\boldsymbol{\beta}^{-10}$ are identical except for the elements $\beta^{10}_{01} = \beta^{10}_{10} = -\beta^{-10}_{10} = -\beta^{-10}_{01}$. All other elements different from zero have $i+k$ = even. If now we transform the matrix $\boldsymbol{\beta}^{10}$ with a matrix A with elements

$a_{ik} = (-1)^{i+1}\delta_{ik}$, all elements of $\boldsymbol{\beta}^{10}$ are multiplied by the factor $(-1)^{i+k}$. Consequently we obtain the equivalence

$$\boldsymbol{\beta}^{-10} = A\boldsymbol{\beta}^{10}A^{-1}. \tag{6.27}$$

Appendix 3

BASIS FUNCTIONS OF THE REPRESENTATIONS [3,1] AND [2,1²] FOR FOUR PARTICLES

The functions $[3,1]_j, j = 1, 2, 3$ of sect. 6(e) are basis functions of the representation $\bar{D}^{[3,1]}(S_4)$ spanned by $\ddot{\boldsymbol{\eta}}^1, \ddot{\boldsymbol{\eta}}^2, \ddot{\boldsymbol{\eta}}^3$. The transformations of these vectors under permutations are given in table 3, and we conclude from it that

$$\begin{aligned}(1,4)[3,1]_3 &= -[3,1]_2,\\ (1,3)[3,1]_3 &= -[3,1]_1,\end{aligned} \tag{A.6}$$

which allows us to obtain $[3,1]_2$ and $[3,1]_1$ including phases from $[3,1]_3$. With the results of table 3 we find explicitly

$$\begin{aligned}\langle\kappa\lambda\mu'|(1,4)|\kappa\lambda\mu\rangle &= (-1)^\kappa i^{\mu'+\mu} d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi),\\ \langle\kappa\lambda\mu'|(1,3)|\kappa\lambda\mu\rangle &= (-1)^\kappa(-1)^\mu d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi),\end{aligned} \tag{A.7}$$

or

$$\begin{aligned}\langle\kappa\lambda\rho'|\mu'||(1,4)|\kappa\lambda\rho|\mu|\rangle &= (-1)^\kappa g_{\mu'\mu}(i^{\mu'+\mu}+\rho i^{-\mu'-\mu})d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi)\delta_{\rho'\rho}\\ \langle\kappa\lambda\rho'|\mu'||(1,3)|\kappa\lambda|\mu|\rangle &= (-1)^\kappa\tfrac{1}{2}[(-1)^\mu+\rho'+\rho(-1)^{\mu'-\mu}+(-1)^{\mu'}\rho'\rho]d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi)\\ &\qquad\times i^{\frac{1}{2}(\rho-\rho')+\mu-\mu'}.\end{aligned} \tag{A.8}$$

By projection technique we find that all basis functions $[3,1]_3$ have $\varepsilon = \pm 1, \rho = -1$ and may be distinguished by $|\mu|$. Consequently using (A.6) and (A.7) we find, for fixed even $|\mu|$:

$$[3,1]_2 = -\sum_{|\mu'|}|\kappa\lambda\rho|\mu'|\rangle(-1)^\kappa g_{\mu'\mu}[1-(-1)^{\mu'}]d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi), \tag{A.9}$$

which shows that all $[3,1]_2$ functions have $\varepsilon = 0$, $\rho = -1$. Similarly

$$[3,1]_1 = -\sum_{|\mu'|}|\kappa\lambda\rho|\mu'|\rangle(-1)^\kappa[1-(-1)^{\mu'}]d^\lambda_{\mu'\mu}(\tfrac{1}{2}\pi)i^{\mu-\mu'-1}, \tag{A.10}$$

where $\rho\rho' = -1$ or $\rho' = +1$, $\varepsilon'(\mu') = 0$ in agreement with table 5.

The basis functions for the representation [2, 1, 1] of S_4 may be obtained on replacing $\ddot{\boldsymbol{\eta}}^1, \ddot{\boldsymbol{\eta}}^2, \ddot{\boldsymbol{\eta}}^3$ by three quantities which are unchanged under the inversion I. The corresponding representation $\bar{D}^{[2,1,1]}(S_4)$ is obtained from $\bar{D}^{[3,1]}(S_4)$ by omitting all inversions. Consequently

$$\begin{aligned}(1,4)[2,11]_2 &= [2,11]_2,\\ (1,3)[2,11]_3 &= [2,11]_1,\end{aligned} \tag{A.11}$$

$$[2, 1, 1]_2 = \sum_{|\mu'|} |\kappa\lambda\rho|\mu'|\rangle g_{\mu'\mu}[1-(-1)^{\mu'}]d^{\lambda}_{\mu'\mu}(\tfrac{1}{2}\pi). \tag{A.12}$$

$$[2, 1, 1]_1 = \sum_{|\mu'|} |\kappa\lambda\rho|\mu'|\rangle g_{\mu'\mu}[1-(-1)^{\mu'}]d^{\lambda}_{\mu'\mu}(\tfrac{1}{2}\pi)i^{\mu-\mu'-1}, \tag{A.13}$$

where $\rho = -1$, $\varepsilon = \pm 1$ and $\rho' = 1$, $\varepsilon'(\mu') = 0$.

In order to diagonalize X in all the different submatrices $\boldsymbol{\beta}^{\rho\varepsilon}$, it suffices to do this for $\varepsilon = \pm 1$ since the relations (A.9), (A.10), (A.12) and (A.13) give the eigenvectors for $\varepsilon = 0$ in terms of the others. For the representations [3, 1] and [2, 1, 1], the diagonalization of X is, in fact, not necessary since we may use the index $|\mu|$ related to $(\ddot{A}_3)^2$ to distinguish the different functions $[3, 1]_3$ or $[2, 1, 1]_3$ and obtain the partner functions from them.

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