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The unique labelling of states via Mackey's theorem

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Abstract. A new approach to finding unique labels for many-electron states in multicentre systems is described and a particular example (eight electrons in s-states on eight centres) is worked out in detail. This approach is shown to provide a labelling with a more direct physical interpretation than has previously been found.

1. Introduction

This paper is one of a series developing new methods for labelling the states of multicentre systems using the permutation group. The optimal choice of labelling methods is important in the physical interpretation of solutions as well as in the mathematical process of diagonalising Hamiltonians. 'Unique' labelling methods have the property that every state is completely described by a set of irreducible representation labels for groups characterising the system.

The long term aim of this series of papers is to find exact solutions to the generalised Hubbard model for a variety of systems with a finite number of centres. These solutions can then be used as a test of approximative methods and to determine the forms of model Hamiltonian which most adequately describe electron localisation and intermediate valence phenomena.

Unique labelling in terms of the irreducible representation labels for a chain of groups depends on unique labelling for every group/subgroup link in the chain. This holds when the subduction (or reduction) of every irreducible representation of the group corresponds to a combination of irreducible representation labels of the subgroup *with no repeats.* The power of this method is considerably enhanced by the reciprocity theorem due to Frobenius (e.g. see Ledermann 1977, p 74), which states that the correlation tables for induced representations are the same as those for subduced representations. Hence unique labelling by subduction implies unique labelling by induction. In practice the choice between these procedures will be determined by which group in the chain is used to characterise the physical basis vectors.

In a recent paper (Chan and Newman 1983, henceforth referred to as paper II) it has been shown possible to obtain a unique group theoretical labelling of all the many electron states generated by $l(<2n)$ electrons in s-states on n centres. S_n and its permutation subgroups were used in this labelling. Furthermore, it was shown possible, by introducing subgroup chains relating spatial symmetry groups to S_8, to obtain unique labels for all the states for systems where eight centres are fixed in cyclic regions (Chan and Newman 1982, henceforth referred to as paper I) or rigid isolated systems.

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A feature of the above approach to S_n labelling is that comparisons were made between a combinatoric method based on Polya's theorem (Newman 1982) and a purely group theoretical method based on induced representation theory. Although the combinatoric method was shown to lead to a correct *enumeration* of the states (for $n = 8$), it did not provide sufficient information for a unique labelling. The main problem with this approach is that it classifies states (colourings or other structures defined on the lattice) as equivalence classes of S_n, which may then be difficult to resolve uniquely into equivalence classes of the spatial symmetry group (e.g. see the discussion in Newman (1982) and in § 4 of this work).

In this paper we shall present a third approach to this same problem which is as powerful as the induced representation approach and yet provides the heuristic advantage, characteristic of the combinatorial method, of identifying equivalence class groups. The relationship between the induced representation approach and our present techniques is shown symbolically in figure 1. The group S_n is decomposed into double cosets HdK, where the d's are a set of elements of S_n (called 'double coset representatives') chosen so that the corresponding set of double cosets spans all the elements in S_n. In II we labelled the states spanned by S_n by first inducing representations of H into S_n to provide a unique labelling of the S_n states, and then subducing these into K. Here we shall first obtain the set of intersection groups L^d and then determine the subduced representation labels for the chains $H^d \supset L^d$ and $K \supset L^d$ (with suitable intermediate groups).

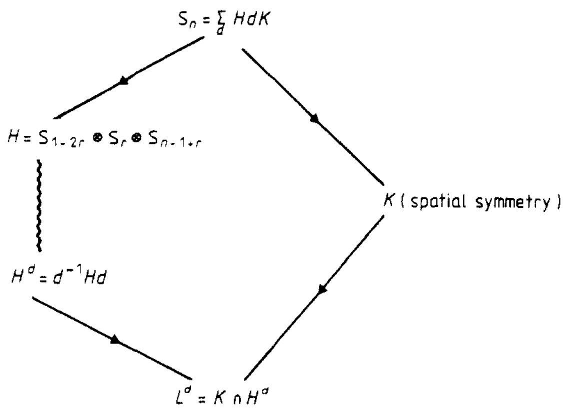

Figure 1. Subgroup relations relevant to the application of Mackey's theorem.

From the combinatoric point of view each total spin state S and M_S value of a configuration of states is regarded as a 'structure' defined on the n centres. Any state of the configuration (with given S, M_S) may be transformed into any other state with the same S, M_S values under S_n. Hence the set of all states of a configuration with given S, M_S may be regarded as a single equivalence class with respect to S_n. This generalises the classical notion of an equivalence class because the antisymmetry of the states under particle exchange leads us to introduce negative characters (as in II, table 2). In Newman (1982) it was remarked that every equivalence class could be related to the subgroup which left the structure generating the equivalence class invariant. The configuration groups are seen to fulfil this role in the present work for equivalence classes with respect to S_n, although we do not restrict ourselves to the identity representation of the configuration groups as is done in simple colouring problems.

A single equivalence class with respect to S_n will generally break into several equivalence classes with respect to its subgroups and, in particular, with respect to those subgroups which correspond to rigid spatial (or cyclic region) arrays of the n centres. As was remarked by Newman (1982), it is far from trivial to determine the way in which equivalence classes with respect to S_n break down into equivalence classes with respect to spatial symmetry subgroups of S_n. The equivalence class groups generated by the total spin eigenstate configurations of eight electrons in s-states on eight centres will be the focus of our present investigation. We note that they can be identified with the groups L^d of figure 1, for these are the possible intersection groups between the configuration groups H^d and the spatial symmetry group K.

2. General formulation

The method we shall use is based on Mackey's theorem (Altmann 1977) and is related to the use of this theorem in labelling suggested by Newman (1983). Given the double coset decomposition of S_n,

$$S_n = \sum_d HdK, \tag{2.1}$$

where the symbols have the interpretation given in the previous section, Mackey's theorem relates the representations as follows:

$$(\Delta \uparrow G)\downarrow K = \sum_d (\Delta^d \downarrow L^d)\uparrow K \tag{2.2}$$

where $\uparrow$, $\downarrow$ represent induction and subduction, Δ is a representation of H and $\Delta^d(d^{-1}hd) = \Delta(h)$, $h \in H$. Equation (2.2) neatly relates the paths in figure 1 used in our previous labelling scheme (on the left-hand side) with those we shall use in the present approach (on the right-hand side).

In our new approach the first problem to be solved is to determine the set of groups $L^d = K \cap H^d$ corresponding to the intersection of the configuration symmetry (H^d) and the spatial symmetry K. This problem is best solved in non-trivial cases by symbolic computation (see the appendix). Character tables then have to be established for the groups L^d. There must then be chains of intermediate groups between L^d and H^d and between L^d and K in order to ensure unique labelling for the subduction and induction processes on the right-hand side of (2.2).

3. A worked example: eight electrons on eight sites

We shall presume that the spatial symmetry of the eight sites is given by the 192-element cyclic region group described in I and denoted here by G(192).

It may also be of interest to the reader that the 384-element group called $O^5/2FCC$ in I is mentioned (among others) in the work of Koptsik and Evarestov (1980) as an 'extended unit cell group'. A distinct 384-element cyclic region group with 20 classes also mentioned in that paper (as a factor group of O_h^7) is isomorphic with the hyper-octahedral group which has the character table given by Baake *et al* (1982).

We shall adopt the same notation for the irreducible representations of G(192) as was employed in I and shall not reproduce the character table here. Note that many other spatial symmetries correspond to subgroups of G(192), so that a solution for G(192) can be used to provide a range of other solutions.

The elements of G(192) will be described using a two-number notation in which the first number denotes one of the 24 rotations defined by figure 2 and table 1, and the second is one of the eight cyclic translations defined by the centre labels in the same figure. For example, $\boldsymbol{t}_2 \equiv (1, 2)$ denotes a translation from centre 1 to centre 2 (or a parallel translation of the same magnitude). In particular, $\boldsymbol{t}_1 \equiv (1, 1)$ is the identity operation. We shall identify the intersection groups L^d with a set of elements given in this notation.

As discussed in II there are five configurations for a system with eight electrons on eight sites according to whether no pairing of up and down spin electrons on a given site occurs (with configuration group S_8), one such pair occurs ($S_1 \otimes S_1 \otimes S_6$), two pairs occur ($S_2 \otimes S_2 \otimes S_4$), three pairs occur ($S_3 \otimes S_3 \otimes S_2$) or all eight electrons are

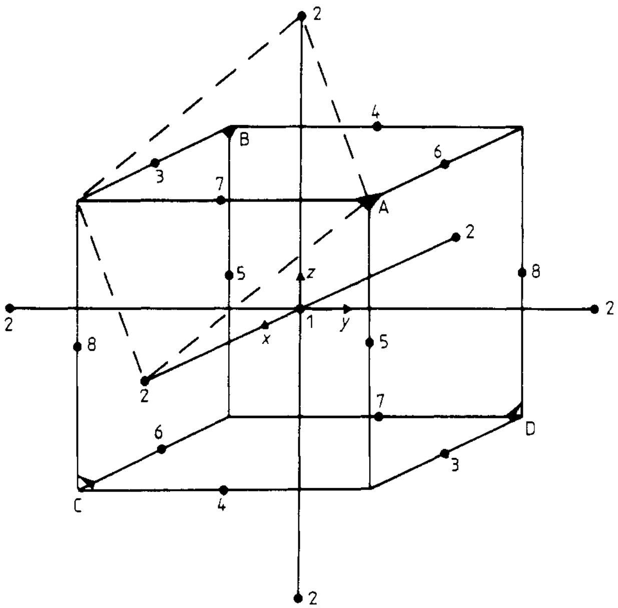

Figure 2. The eight distinct atoms in the cyclic region are shown together with labelling of rotation axes used in this work. Translations are labelled relative to the atomic positions relative to the central atom 1.

Table 1. Dictionary for the numerical labelling of the elements of the octahedral group. The axis labels are shown in figure 2.

Label	1	2	3	4	5	6	7	8
Rotation	E	C_{2x}	C_{2y}	C_{2z}	C_{4x}^+	C_{4x}^-	C_{4y}^+	C_{4y}^-
Label	9	10	11	12	13	14	15	16
Rotation	C_{4z}^+	C_{4z}^-	C_{3A}^+	C_{3A}^-	C_{3B}^+	C_{3B}^-	C_{3C}^+	C_{3C}^-
Label	17	18	19	20	21	22	23	24
Rotation	C_{3D}^+	C_{3D}^-	$C_2'(5)$	$C_2'(8)$	$C_2'(7)$	$C_2'(6)$	$C_2'(4)$	$C_2'(3)$

paired ($S_4 \otimes S_4$). The groups L^d for each of these configurations have been calculated using the methods described in the appendix. Symbols for the groups L^d are defined in terms of their elements below and table 2 relates to isomorphic point groups.

Table 2. Complete list of the groups L^d for all configurations of eight electrons in s-states on eight centres. Identifications are given with point groups, daggers indicating isomorphism but not physical equivalence. Coloration symbols denote the effect of the transformation $d^{-1}(S_u \otimes S_u \otimes S_{8-2u})d$, e.g. for G_2, $d^{-1}(S_2\{12\} \otimes S_2\{34\} \otimes S_4\{5678\})d = S_2\{12\} \otimes S_2\{36\} \otimes S_4\{5478\}$ denoted by $\{12\}\{36\}\{5478\}$.

Configuration group	L^d group		$\lvert L^d \rvert$	Coloration	References
S_8	G (192)	G (192)	192	{12345678}	Chan and Newman (1982)
$S_1 \otimes S_1 \otimes S_6$	F_1	O	24	{1}{2}{345678}	—
	F_2	D_2'	4	{1}{3}{245678}	—
$S_2 \otimes S_2 \otimes S_4$	G_1	$D_2^\dagger$	4	{12}{34}{5678}	—
	G_2	$D_4 \otimes \{E, t_2\}$	16	{12}{36}{5478}	as for $D_4 \otimes C_s$
	G_3	C_1	1	{13}{24}{5678}	—
	G_4	$D_2 \otimes \{E, t_3\}$	8	{13}{26}{4578}	as for $D_2 \otimes C_s$
	G_5	$D_2^\dagger$	4	{13}{45}{2678}	—
	G_6	$D_2^\dagger$	4	{13}{47}{5628}	—
	G_7	$C_2 \otimes \{E, t_3\}$	4	{13}{48}{2567}	as for D_2
$S_3 \otimes S_3 \otimes S_2$	H_1	$C_2^\dagger$	2	{123}{456}{78}	—
	H_2	$C_2^\dagger$	2	{123}{457}{68}	—
	H_3	$D_2^\dagger$	4	{123}{467}{58}	—
	H_4	$C_2^\dagger$	2	{134}{256}{78}	—
	H_5	$C_2^\dagger$	2	{134}{258}{67}	—
	H_6	$D_3^\dagger$	6	{134}{267}{58}	—
	H_7	$C_2^\dagger$	2	{134}{268}{57}	—
$S_4 \otimes S_4$	I_1	$D_2^\dagger$	4	{1234}{5678}	—
	I_2	$D_4 \wedge \{E, t_2, t_3, t_6\}$	32	{1236}{5478}	Table 3
	I_3	$O^\dagger$	24	{1345}{2678}	—
	I_4	$D_3 \otimes \{E, t_3, t_4, t_8\}$	24	{1348}{2567}	as for O

3.1. *Configurations S_8*

As $S_8 \supset G(192)$, G(192) itself is the only L^d group.

3.2. *Configurations $S_1 \otimes S_1 \otimes S_6$*

The double coset decomposition involves two groups which will be denoted F_1 and F_2. Both groups do not contain any cyclic translations and we can identify $F_1 = O$ (as defined by figure 2) and $F_2 = \{(1,1), (2,1), (22,1), (24,1)\} = D_2'$. Here the prime distinguishes a subgroup of O containing two C_2' axes.

3.3. *Configurations $S_2 \otimes S_2 \otimes S_4$*

In this case the double coset decomposition requires seven groups as follows:

$G_1 = \{(1,1), (4,2), (19,2), (20,1)\}$

$G_2 = \{(1,1), (1,2), (2,1), (2,2), (3,1), (3,2), (4,1), (4,2), (5,1), (5,2),$
$(6,1), (6,2), (22,1), (22,2), (24,1), (24,2)\} \equiv D_4 \otimes \{E, t_2\}$

$G_3 = (1,1) \equiv C_1$

$G_4 = \{(1,1), (1,3), (2,1), (2,3), (22,1), (22,3), (24,1)\ (24,3)\} \equiv D_2 \otimes (E, t_3)$

$G_5 = \{(1,1), (2,3), (22,1), (24,3)\}$

$G_6 = \{(1,1), (2,1), (22,3), (24,3)\}$

$G_7 = \{(1,1), (1,3), (24,1), (24,3)\} \equiv C_2 \otimes \{E, t_3\}.$

3.4. *Configuration* $S_3 \otimes S_3 \otimes S_2$

In this case there are given seven groups in the double coset decomposition:

$H_1 = \{(1,1), (22,1)\}$

$H_2 = \{(1,1), (3,2)\}$

$H_3 = \{(1,1), (2,1), (3,2), (4,2)\}$

$H_4 = \{(1,1), (24,3)\}$

$H_5 = \{(1,1), (20,1)\}$

$H_6 = \{(1,1), (11,3), (12,4), (20,1), (23,4), (24,3)\}$

$H_7 = \{(1,1), (24,3)\}.$

3.5. *Configuration* $S_4 \otimes S_4$

The double coset decomposition requires only four groups in this case:

$I_1 = \{(1,1), (4,2), (19,2), (20,1)\}$

$I_2 \doteq D_4 \wedge (E, t_2, t_3, t_6),$

where D_4 is identical to that defined by the list of elements for G_2

$I_3 = \{(1,1), (2,3), (3,4), (4,5), (5,4), (6,5), (7,5), (8,3), (9,4), (10,3),$
$(11,3), (12,4), (13,1), (14,1),$
$(15,3), (16,5), (17,4), (18,5), (19,5),$
$(20,1), (21,1), (22,1), (23,4), (24,3)\}$

$I_4 = \{(1,1), (1,8), (1,4), (1,3), (11,1), (11,8), (11,4), (11,3), (12,1), (12,8),$
$(12,4), (12,3), (20,1), (20,8), (20,4), (20,3), (23,1), (23,8),$
$(23,4), (23,3), (24,1), (24,8), (24,4), (24,3)\}$
$\equiv D_3 \otimes \{E, t_3, t_4, t_8\}.$

Chains of subgroups relating all these groups with G(192) are shown in figure 3. In most cases the character tables of these groups are well known because of isomorphisms with the point groups. An exceptional case is I_2, and the character table for this group is given in table 3. Using the character tables we are then able to generate correlation relations, the most important of which are given in tables 4–8. These show that the reduction $\Delta^d \downarrow L^d$ of (2.2) can be labelled uniquely in this configuration.

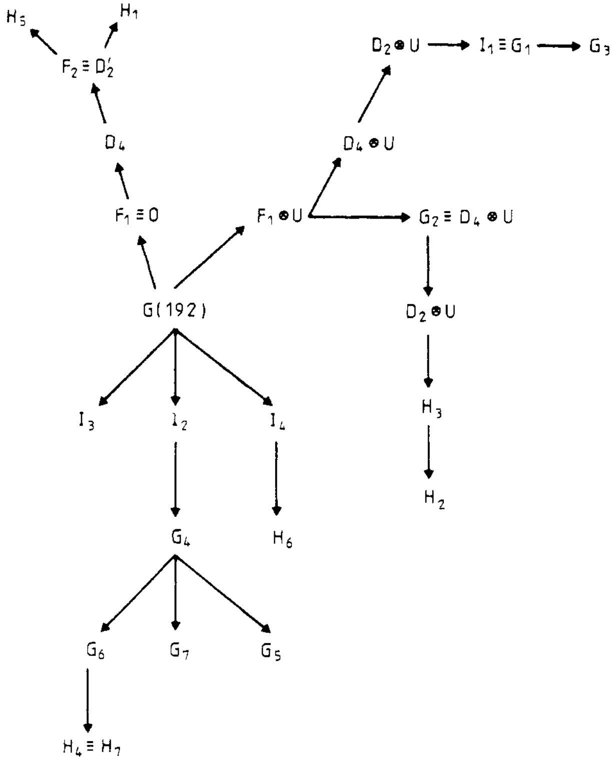

Figure 3. Subgroup relations between groups listed in table 1. The group $U = \{E, t_2\}$. Other groups are defined in table 1 and in the text. D_4 is assumed to have its C_4 axis aligned in the x direction, while D_4' has a z alignment. Correlation tables 4–7 show that the group/subgroup relations in this figure provide a unique labelling of the G(192) representations of all states of the eight-electron system.

The remaining problem is to find a unique labelling scheme for the group/subgroup chains connecting the configuration groups $S_u \otimes S_u \otimes S_{8-2u}$ with the L^d. The states to be considered can be derived from the columns of table 1 of II with $n = 8 - 2u = 8$, 6, 4, 2 and 0.

3.6. *Configuration S_8*

In this case it is necessary to find a chain of groups relating S_8 to G(192) which allows for a unique labelling of the S_8 representations of interest as identified by the $n = 8$ column in table 1 of II. A general solution of this labelling problem was given in I by introducing as intermediate groups the alternating group A_8 and the subgroup $[8]+[4^2]+[2^4]+[1^8]$ (in the notation of Littlewood (1958, appendix)). As this was the least straightforward problem to solve using the previous method, it cannot be claimed that the present approach simplifies the analysis.

Table 3. Character table for the group $I_2 = D_4 \wedge (E, t_2, t_3, t_6)$. Class labels are defined by figure 2 with the C_4 axis in the x direction and as follows. $\boldsymbol{t}(=t_2)$ is a translation along the C_4 axis; $\boldsymbol{t}_b(=t_3$ or $t_6)$ is a translation in the 'basal plane', perpendicular to the C_4 axis; $C_2 = C_4^2$; C_{2b} is about an axis in the basal plane in the primitive vector direction; C'_{2b} is about axes at 45° to the C_{2b} in the basal plane. $C_{2b}\boldsymbol{t}_b^{\parallel}$ has $\boldsymbol{t}_b$ and the C_2 axis parallel, while $C_{2b}\boldsymbol{t}_b^{\perp}$ has them perpendicular. $C_4\boldsymbol{t}$ and $C'_{2b}\boldsymbol{t}$ each have two members corresponding to pure rotations, and two combining these with $\boldsymbol{t}$.

Class	E	C_2	$C_2\boldsymbol{t}$	$C'_{2b}\boldsymbol{t}$	C_{2b}	$C_{2b}\boldsymbol{t}^{\parallel}$	$\boldsymbol{t}_b$	$C_2\boldsymbol{t}_b$	$C_{2b}\boldsymbol{t}_b$	$C_{2b}\boldsymbol{t}_b^{\perp}$	$\boldsymbol{t}$	$C_{2b}\boldsymbol{t}_b$	$C_4\boldsymbol{t}$	$C_4\boldsymbol{t}_b$
Order	1	1	1	4	2	2	2	2	2	2	1	4	4	4
(D_4) A_1^{Γ}	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_2^{Γ}	1	1	1	−1	−1	−1	1	1	−1	−1	1	−1	1	1
B_1^{Γ}	1	1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
B_2^{Γ}	1	1	1	−1	1	1	1	1	1	1	1	−1	−1	−1
E^{Γ}	2	−2	−2	0	0	0	2	−2	0	0	2	0	0	0
(D_4) A_1^{M}	1	1	1	1	1	−1	−1	−1	1	−1	1	−1	1	−1
A_2^{M}	1	1	1	−1	−1	1	−1	−1	−1	1	1	1	1	−1
B_1^{M}	1	1	1	1	−1	1	−1	−1	−1	1	1	−1	−1	1
B_2^{M}	1	1	1	−1	1	−1	−1	−1	1	−1	1	1	−1	1
E^{M}	2	−2	−2	0	0	0	−2	2	0	0	2	0	0	0
(D_2) A_1^{R}	2	2	−2	0	2	0	0	0	−2	0	−2	0	0	0
B_1^{R}	2	2	−2	0	−2	0	0	0	2	0	−2	0	0	0
B_2^{R}	2	−2	2	0	0	2	0	0	0	−2	−2	0	0	0
B_3^{R}	2	−2	2	0	0	−2	0	0	0	2	−2	0	0	0

3.7. Configuration $S_1 \otimes S_1 \otimes S_6$

The S_6 representations may be reduced with respect to the octahedral group $F_1 \equiv O$ by noting the following correspondence between classes (see figure 2):

$$\begin{array}{llllll} S_6 \text{ classes:} & 1^6 & 1^2 2^2 & 1^2 4 & 3^2 & 2^3 \\ O \text{ classes:} & E & C_2 & C_4 & C_3 & C'_2. \end{array}$$

Comparison of the character tables then gives the following subductions of the configuration group representations:

$$[2^3] \to A_1 + A_2 + T_2 \qquad [2^2 1^2] \to A_1 + E + T_1 + T_2$$

$$[21^4] \to E + T_2 \qquad [1^6] \to A_1.$$

In the case $F_2 \equiv D'_2$ a direct correlation between the irreducible representations does not lead to a unique labelling. We may, however, introduce an intermediate octahedral group which will enable a unique labelling to be made following the chain

$$S_1(1) \otimes S_1(3) \otimes S_6(2\,4\,5\,6\,7\,8) \supset O' \supset D'_2.$$

In this equation O' is the transform of O produced by interchanging the centre labels 2 and 3. We may then use the correlations given above for the first link in the chain and table 4 of I for the second link.

3.8. Configuration $S_2 \otimes S_2 \otimes S_4$

Correlation relations for all the L^d groups of this configuration are given in table 4. This table shows that all reductions are unique except for the case of G_3 and G_4, so

Table 4. Correlation relations for L^d groups of the configuration $S_2 \otimes S_2 \otimes S_4$. Bracketed (isomorphic) groups indicate the irreducible representation labelling that is employed.

S_4 representation:	$[2^2]$	$[21^2]$	$[1^4]$
G_1, G_6 and $G_9(D_2)$	A_1+B_2	$B_1+B_2+B_3$	B_2
$G_2(D_4 \otimes C_s)$	$A_{1g}+B_{2g}$	E_u+A_{2g}	B_{2g}
$G_4(D_2 \otimes C_s = D_{2h})$	$2A_{1g}$	$B_{1u}+B_{2u}+B_{3g}$	A_{1g}
$G_5(D_2)$	A_1+B_1	$B_1+B_2+B_3$	B_1

that further consideration will only be given to these two cases. We are interested in the action of this group on the four centre labels 4578 which are permuted by S_4 (see table 2). In this case the elements (1, 3) and (24, 1) (for example) of G_4 cannot be distinguished, both corresponding to the permutation (48)(57). We therefore find that G_4 reduces to a group G_4' which is isomorphic to D_2 when acting on the centre labels 4578, namely

$$G_4'\text{: } (4)(5)(7)(8),\ (47)(58),\ (45)(78),\ (48)(57).$$

We are therefore concerned to find a group intermediate between this group and S_4. A suitable group is obtained by introducing the additional elements (48)(5)(7), (57)(4)(8), (4785) and (4587) giving a group isomorphic to D_{2d} which may be related to S_4 through its isomorphism to T_d. The appropriate correlations are shown in table 5.

Finally we note that all the representations of C_1 can be labelled uniquely by using the sequence $C_1 \subset D_2' \subset S_4$, where the relation between D_2' and S_4 is isomorphic to that between G_1 and S_4 (see table 3).

Table 5. Correlation table for G_4 using an intermediate group isomorphic to D_{2d} (see text).

S_4/T_d	D_{2d}	$G_4(D_2)$
$[2^2]/E$	A_1+B_1	$(A_1)A_1+B_1(A_1)$
$[21^2]/T_1$	$E+A_2$	$(E)B_1+(E)B_2+(A_2)B_3$
$[1^4]/A_1$	A_1	$(A_1)A_1$

3.9. *Configuration $S_3 \otimes S_3 \otimes S_2$*

In this case there are only two one-dimensional representations of S_2 to consider. Their reductions with respect to the groups H_i are shown in table 6. There are no problems with unique labelling as the S_2 representation labels are themselves unique.

Table 6. Correlation table for the group H_i.

S_2	$H_1(C_2)$	$H_2(C_2)$	$H_3(D_2)$	$H_4(C_2)$	$H_5(C_2)$	$H_6(D_3)$	$H_7(C_2)$
[2]	A	A	A_1	A	A	A_1	A
$[1^2]$	B	A	B_2	A	B	A_1	A

3.10. Configuration $S_4 \otimes S_4$

The $[4]\otimes[4]$ representation is one-dimensional, so that no labelling problems arise.

4. A comparison of methodology

In this section we shall compare the labelling schemes for eight electrons in s-states on eight centres developed in II with that developed in the present work. For this purpose it will be sufficient to compare these approaches for the configuration $1^6 2$. According to table 3 of II there are 3584 states in this configuration. A combinatoric method was used to obtain the S_8 characters for these states corresponding to their M_S values (see table 2 of II). This method was based on looking at the possible ways of 'colouring' a certain number of centres with labels corresponding to the spin arrangement on each centre, etc (i.e. $a \equiv \uparrow$, $b \equiv \downarrow$, $c \equiv \uparrow\downarrow$). In fact the combinatorial results in table 2 of II can readily be obtained by inducing the identity representation of the 'colouring' group $S_\alpha \otimes S_\beta \otimes S_\gamma \otimes S_{8-\alpha-\beta-\gamma}$ where α is the number of a labels, β the number of b's and γ the number of c's. These colouring groups are in fact subgroups of the configuration groups $S_{\alpha+\beta} \otimes S_\gamma \otimes S_{8-\alpha-\beta-\gamma}$ used in the group theoretical approach of II.

In order to cope with the antisymmetry of electrons under interchange a rather *ad hoc* extension of the combinatorial procedure was introduced in II. This can easily be shown to correspond to inducing the representation $[1^\alpha]\otimes[1^\beta]\otimes[\gamma]\otimes[8-\alpha-\beta-\gamma]$ rather than the identity representation $[\alpha]\otimes[\beta]\otimes[\gamma]\otimes[8-\alpha-\beta-\gamma]$.

With this reformulation of the combinatoric method in group theoretical terms it becomes easy to obtain unique labels for the irreducible representations corresponding to M_S labels. We simply insert the same series of intermediate groups that was used in the group theoretical (i.e. configuration group) approach in II, namely

$$S_n \supset S_m \otimes S_{n-m} \supset S_m \otimes S_\gamma \otimes S_{n-\gamma-m} \supset S_\alpha \otimes S_\beta \otimes S_\gamma \otimes S_{n-\alpha-\beta-\gamma}$$

where $m = \alpha + \beta$.

It would also be possible to apply Mackey's theorem if the group H was identified with a colouring group, although it is clear that the equivalence class groups L^d then obtained would be subgroups of the L^d obtained in this work. As M_S labelling is usually of less interest than the S, M_S labelling we shall not pursue this matter here. Nevertheless, it should be pointed out that this approach provides a feasible way of overcoming the difficulties encountered in the work of Newman (1982), where the characters of an S_6 colouring were found insufficient in themselves to determine the equivalence class groups for six centres in an octahedral array.

The group theoretical method used in II bypasses this problem, using the induced representations of the chain

$$S_8 \supset S_1 \otimes S_7 \supset S_1 \otimes S_1 \otimes S_6 \tag{4.1}$$

to specify unique labels for all the S_8 states of the configuration $1^6 2$ listed in table 3 of II. This approach also provides a method of generating table 3 of II without first obtaining table 2 of II combinatorially. The $2^6 = 64$ states of 1^6 induce $64 \times 8!/6! = 3584$ states of $1^6 2$. Unique labelling genealogies are given in figures 1 and 2 of II.

In the present work we again begin with the 64 states of the configuration 1^6. If we identify $G \equiv S_8$ and $H \equiv S_1 \otimes S_1 \otimes S_6$ in (2.2), the expression $\Delta \uparrow G$ corresponds to the process of inducing these 64 states into S_8 to produce the 3584 states of the configuration $1^6 2$. $(\Delta \uparrow G)\downarrow K$ therefore corresponds to the subduction of these states with respect to the spatial symmetry group, here identified as G(192). The right-hand side of (2.2), which we have been using, first requires the identification of the groups L^d which, according to table 2, may be identified as $F_1 \equiv O$ and $F_2 \equiv D_2'$ in the present case.

The 64 states of 1^6 are spanned by the representations $[2^3]$ $(S=0)$, $[2^2 1^2]$ $(S=1)$, $[21^4]$ $(S=2)$ and $[1^6]$ $(S=3)$. These are subduced into O and D_2' as shown in table 7.

Table 7. Subduction of S_6 representations into O and D_2' and induction of O representations into G(192).

Total spin	S_6 representations	O representations	D_2' representations	$O\uparrow G(192)$ representations
$S=0$	$[2^3]$	A_1	A_1	$A_1^\Gamma + A_1^X + A_1^L$
		A_2	B_1	$A_2^\Gamma + B_1^X + A_2^L$
		T_2	$A_1+B_2+B_3$	$T_2^\Gamma + B_2^X + E^X + A_1^L + E^L$
$S=1$	$[2^2 1^2]$	A_1	A_1	$A_1^\Gamma + A_1^X + A_1^L$
		E	A_1+B_1	$E^\Gamma + B_1^X + A_1^X + E^L$
		T_1	$B_1+B_2+B_3$	$T_1^\Gamma + A_2^X + A_1^X + E^L$
		T_2	$A_1+B_2+B_3$	$T_2^\Gamma + B_2^X + E^X + A_1^L + E^L$
$S=2$	$[21^4]$	E	A_1+B_1	$E^\Gamma + B_1^X + A_1^X + E^L$
		T_2	$A_1+B_2+B_3$	$T_2^\Gamma + B_2^X + E^X + A_1^L + E^L$
$S=3$	$[1^6]$	A_1	A_1	$A_1^\Gamma + A_1^X + A_1^L$

According to (2.2) the representations of G(192) induced by these two sets of representations (for D_2' and O) will span the complete set of 3584 states of $1^6 2$. Given that O contains 24 elements and D_2' contains 4 elements we see that this corresponds to the breakdown

$$3584 = 64\times 192/24 + 64\times 192/4. \tag{4.2}$$

A typical state labelling for an $S=2$ state with $L^d = D_2'$ would thus be (see table 7):

$$[21^4],\ T_2,\ A_1;\ E,\ B_1^X$$

corresponding to the sequence

$$[21^4]\downarrow O\downarrow D_2'\uparrow O\uparrow G(192). \tag{4.3}$$

It will be noted that there is no 1–1 correspondence between the labels obtained in this way and the $S_1\otimes S_1\otimes S_6\uparrow S_8\downarrow G(192)$ labels obtained in II, apart from their common generation from states of the 1^6 configuration.

Finally we note that groups O and D_2' have a simple geometrical interpretation in terms of figure 2 with the colorations corresponding to F_1 and F_2 shown in table 2. In the case of F_1 centres, 1 and 2 occupy fixed positions, allowing all the operations of the octahedral group O on the remaining six centres (labelled 3 to 8). In the case of F_2, the fixed centres are 1 and 3, allowing only the operations E, $C_2'(3)$, $C_2'(6)$ and C_{2x} in the group D_2'. Unlike a (combinatorial) coloration problem, we are not simply interested in inducing the invariant representations of D_2' and O into G(192), and the present problem involves the induction of all the 64 states of the configuration 1^6 shown in the third and fourth columns of table 7. It will be apparent from the above discussion that O and D_2' are equivalence class groups of G(192), not of S_8.

5. Conclusion

It will be clear from the foregoing example that our method of labelling states using Mackey's theorem requires considerably more effort than the unique labelling scheme derived in II. Nevertheless, the identification of intersection groups (by the method described in the appendix) has considerable heuristic advantages in that it unites the group theoretical and combinatorial points of view.

The calculation of matrix elements using the formalism described in this paper may necessitate the generation of tables of coupling coefficients for the chains of groups considered in this work. However, the work of Seligman (1979) suggests that such tabulations could be bypassed.

Appendix. Determination of the intersection groups L^d

The main problem to be solved in finding the L^d is to construct the double coset decomposition $S_n = \Sigma_d HdK$ for the space group K and various choices of configuration group $H^d = d^{-1}Hd$. It is, however, relatively easy to obtain the right coset decomposition $S_n = \Sigma_r Hr$ by direct tests with various $r \in S_n$, $r \notin H$. Supposing that a set of right coset representatives is known, it can be shown that Hr_1 and Hr_2 belong to the same double coset if, for some $h \in H$, $k \in K$,

$$hr_1 = r_2k. \tag{A1}$$

Hence a simple, if somewhat lengthy method of finding all the double cosets is to first derive the right cosets and then use equation (A1) to group these into double cosets.

There are an equal number of right coset representatives and distinct subgroups $H^r = r^{-1}Hr$ of S_n, each subgroup corresponding to a distinct 'coloration' (as defined in the caption to table 2). For example, in the case of the configuration $H = S_1 \otimes S_1 \otimes S_6$ the coloration {1}{2}{345678} varies according to which two centre labels are in the first two brackets. There are $8 \times 7 = 56$ such colorations, corresponding to $|S_8|/|S_6|$, and therefore 56 right cosets of $S_1 \otimes S_1 \otimes S_6$ in S_8.

Equation (A1) can then be used to relate 8 of these right cosets into the single double coset denoted in table 2 by the subgroup O and the remaining 48 cosets into the double coset denoted by D_2'. This process was carried out on a computer by simply running through all possible h, k to find which colorations were equivalent.

The speed and storage requirements of the above procedure would make it prohibitive to carry out for n greater than 8. However, sophisticated algorithms have been developed for the generation of double cosets (e.g. see Brown *et al* 1974) and these should make it practicable to study systems with larger numbers of centres.

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