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Symmetry properties of direct sum systems

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Abstract. An interpretation of double coset decompositions of groups is given in terms of the construction of systems from similar disjoint subsystems. A natural labelling scheme is developed for the direct product states of systems of this type, providing an extension of the concept of unique labelling. An application of the decoupling transformation to finite direct sum systems is investigated.

1. Introduction

Many group-theoretical techniques have been developed specifically for the solution of group-theoretical problems, such as the determination of complete sets of irreducible representations. In particular the theory of induced representations has been developed mainly with an eye to finding the irreducible representations of symmetric groups and space (i.e. crystal lattice groups). The motivation of the present work is rather different. We are interested in the role of group-theoretical description in facilitating the solution of dynamical problems. Hence the emphasis will be on the interpretation of mathematical definitions and theorems in physical terms: relevant mathematical proofs can be found in the literature.

We shall focus attention specifically on the symmetry properties of systems which can, at least partially, be decomposed into direct sums of similar disjoint subsystems. To be precise we suppose that the state vectors $|\xi\rangle$ which describe the system can be decomposed as a direct sum of state vectors:

$$|\xi\rangle = \sum_{i,j}{}_{\oplus} |\xi_i^{(j)}\rangle. \tag{1.1}$$

In this equation the $|\xi_i^{(j)}\rangle$ for a given value of j are supposed to correspond to *similar* disjoint subsystems. That is to say, they can be interchanged by symmetry operations of the total system (and necessarily have the same dimensions). In the interests of clarity we shall interpret mathematical results in relation to systems with only one value of j, thus retaining just the summation over i in equation (1.1). Some consequences of including more than one j value will be mentioned in the final discussion.

In the context of direct sum systems we shall find it useful to introduce the mathematical ideas of *double cosets* and *induced representations*. These ideas provide the background to the powerful 'reciprocity theorem' due to Frobenius (1903; see also Ledermann 1977) as well as a series of theorems due to Mackey (1951, 1952, 1953) which have been discussed by Coleman (1968), Ledermann (1977) and Altmann (1977). In this part of the work we shall concentrate on the problem of assigning

unique group-theoretical labels to states of the system, taking the view (following Newman 1981) that this is the fundamental group-theoretical problem in physics, as it provides the best possible starting point from which to determine solutions of the dynamical problem.

In particular, we shall extend our previous work on unique labelling to provide a method of labelling the direct product bases of groups which are not simply reducible. This method is exemplified using representations of the 384-element 'cyclic region' group studied by Chan and Newman (1982). Koptsik and Evarestov (1980, table 1) have listed twelve groups of this type defined in cubic lattices, which they refer to as 'extended unit cell groups'. They also mention some possible areas of application.

Another development of the theory relates to situations where the subsystems can be further subdivided into components. Such subdivisions can sometimes be carried out so that either the subsystems are only weakly interacting or the components (within a subsystem) are weakly interacting. Systems of both types have a much simplified dynamical problem. In the latter case this can be solved by a procedure which (in particular context) has been called the 'decoupling transformation' (Newman 1974a,b). We shall show that this procedure has a wider range of application than has previously been described.

2. Examples of direct sum systems and their group-theoretical description

The symmetry group H of a subsystem is necessarily a subgroup of the group G of operations which leave the complete system invariant. It is also a subgroup of the local group L of an isolated subsystem. The group L becomes important if the subsystems are so weakly interacting that they can be regarded as completely decoupled systems to a good approximation. In this situation the Hamiltonian matrix reduces to a direct sum of intra-subsystem submatrices. Examples of this are the 'superposition model' of crystal fields (Newman 1971) and the 'independent bonding' model used in chemistry. We shall not go into the detailed aspects of this theory, but merely note that the value of the model derives from the fact that L corresponds to a higher symmetry than H.

The symmetry group of the system will generally be denoted G and the subsystem groups will be denoted H_i. The assumption that all subsystems are similar corresponds to the isomorphism of the different H_i. More precisely, the H_i are necessarily conjugate subgroups of G: given any pair of subgroups H_i, H_j we have

$$H_i = gH_jg^{-1}$$

for some element $g \in G$. The H_i are not necessarily distinct for the different subsystems; they cannot be used, in general, to label subsystems.

The precise relationship between subsystems and group operations is best constructed from the 'viewpoint' of a particular subsystem. That is to say, we shall study the process of generating the basis vectors of the complete system $|i, \alpha\rangle$, where i labels the subsystem and α labels the component within the subsystem basis, from the basis $|1, \alpha\rangle$ of a 'home' subsystem. In describing subsystem bases as a whole it will often be convenient to drop the component label α. Writing the home subgroup H_1 we note that its operators map the home basis into itself:

$$H_1|1\rangle \rightarrow |1\rangle.$$

Any operator $g_i \in G$, $g_1 \notin H_1$ will map a home basis vector onto the basis vector of another subsystem. If we span the complete left coset $g_i H_1$ the mapping is between subsystem bases:

$$g_i H_1 |1\rangle \rightarrow |i\rangle.$$

As the left cosets of H_1 in G are disjoint it follows that they are in 1–1 correspondence with the subsystems and thus provide them with unique labels. It also follows that there are just $|G|/|H_1|$ distinct subsystems, where $|G|$ is used to represent the number of elements in G.

Given that $g_i H_1$ generates the basis of the subsystem corresponding to this left coset, we see that *double cosets* $H_1 g_i H_1$ span the subsystem bases which transform into each other under operations in H_1. We can, therefore, classify all subsystems in terms of their relationship with the home subsystem. All *similarly* related subsystems will be included in a basis $H_1 g_i H_1 |1\rangle$ generated by the double coset operators acting on $|1\rangle$. This classification of subsystems is clearly important in relation to the analysis of matrix elements and the description of many-electron states.

It will be apparent from the above argument that double cosets either contain no element in common or are identical. They therefore provide a classification of all the operators in G. A simple formula exists which gives the numbers of operators in each double coset. This is

$$d_i |H_1 g_i H_1| = |H_1|^2 / |\Delta_i| \tag{2.1}$$

where Δ_i is the intersection group $H_1 \cap H_i = H_1 \cap g_1^{-1} H_1 g_i$. Another way of expressing this result, which follows immediately from the discussion of the physical interpretation of double cosets given above, is $|H_1| t$ where t is the number of distinct types of subsystem as classified by their relation to the home system. In specific problems t can usually be obtained by inspection.

From a mathematical point of view, double cosets of the form HgH are a special case of the double cosets HgM where H and M may be different subgroups of G. Such double cosets are relevant if we are studying the relationships between two sets of subsystems, each set having its own distinct symmetry group. This problem has been eliminated from our discussion by the initial assumption that only one set of similar subsystems would be studied.

As a first example we consider the system shown in figure 1. The total symmetry of the system shown is D_{4h} if we assume that the (unspecified) internal structure of

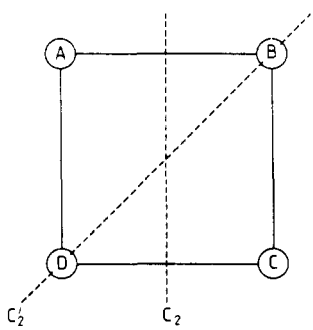

Figure 1. D_{4h} constructed from four equivalent subsystems A, B, C, D. Examples of C_2 and C_2' axes are shown; σ_v and σ_v' planes are perpendicular to these.

the subsystems does not reduce the symmetry of the total system. The subsystems have C'_{2v} symmetry where the C'_2 axis is directed towards the centre of the system. All subsystem subgroups have the operator σ_h in common and pairs of diagonally opposed subsystems have the same symmetry group C'_{2v}.

The two subsystems at corners of the square which are closest neighbours to the home system can be transformed into each other. The intersection group between C_{2v} groups on neighbouring corners is (E, σ_h). All operators which map the home C'_{2v} operators into operators with C'_{2v} groups at the two neighbouring corners make up a double coset with 8 $(=4^2/2)$ elements. Hence, there are just three double cosets in all.

(i) The 'home' (e.g. B) subsystem group $C'_{2v} = C'_{2v}EC'_{2v}$.

(ii) Double cosets relating neighbouring subsystems (e.g. B to C) $C'_{2v}C_4C'_{2v}$.

(iii) The double coset relating opposite subsystems (e.g. B to D) $C'_{2v}C'_2C'_{2v}$.

A second example is provided by the various methods of inducing O_h representations discussed in Newman (1981). If C_{3v} subsystems are used, so that the subsystems are located at each of the eight corners of a cube, there are four double cosets corresponding to an (000), $(a00)$, $(aa0)$ and (aaa) relation between the subsystems (a being the length of a side of the cube). These double cosets have, respectively, 6, 18, 18 and 6 elements, so that together they comprise the 48 elements in O_h.

The work of Newman (1981) and Chen and Newman (1982) makes it clear that there are advantages in choosing subsystems which correspond to Abelian subgroups. An obvious choice for O_h is D'_{2h} which has two C_2 axes of type C'_2 in O_h. In this case there are six subsystems as shown in figure 2 (corresponding to the six cosets of D'_{2h} in O_h). There are, however, only three distinct D'_{2h} subgroups of O_h, and these have no elements other than the identity and inversion in common. Equation (2.1) gives the dimensions of the double cosets as 8, 8 and 32, the latter number indicating that four subsystems bear an equivalent relation to the home subsystem A. In figure 2 these are labelled B, C, D and E.

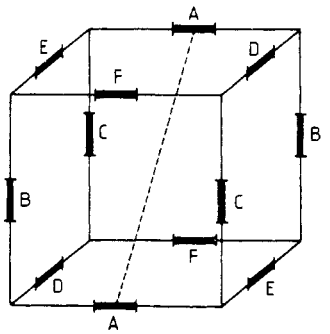

Figure 2. O_h system constructed from six equivalent non-localised subsystems A, B, C, D, E, F. The two parts of the 'home' subsystem A are shown linked.

A third example, which we shall pursue in § 4, is provided by the so-called 'cyclic region group' $O_h^5/(2FCC)$ that has been studied by Chan and Newman (1982). It was remarked in that paper that the chain of groups

$$D'_{2h} \subset O_h \subset O_h^5/(2FCC)$$

provides a unique labelling of the irreducible representations in a 384-dimensional

regular representation of $O_h^5/(2FCC)$. This is demonstrated explicitly by the correlation tables (tables 1 and 2 below) which relate the irreducible representations in the chain, remembering that D_{2h}' is Abelian.

There are three double cosets for $O_h \subset O_h^5/(2FCC)$, corresponding to the relation between an O_h subsystem and itself and the relation between an O_h subsystem and other systems displaced by t and t' (these translations being defined in Chan and Newman (1982, table 5)). The intersection groups corresponding to these double cosets are

$$O_h,\ O_h \cap (t'^{-1} O_h t'),\ O_h \cap (t^{-1} O_h t) = D_{2h}'.$$

As we have indicated above, irreducible representations of both D_{2h}' and O_h provide for a unique labelling of $O_h^5/(2FCC)$ representations.

Table 1. Irreducible representations in the 192-element group G_P containing the proper operations in $O_h^5/(2FCC)$ corresponding to representations induced by O.

	$T_1\uparrow \otimes T_1\uparrow$	$A_1\uparrow$	$A_2\uparrow$	$E\uparrow$	$T_1\uparrow$	$T_2\uparrow$
A_1^Γ	5	1				
A_2^Γ	2		1			
E^Γ	7			1		
T_1^Γ	8				1	
T_2^Γ	9					1
A_1^X	12	1		1		
A_2^X	8				1	
B_1^X	9		1	1		
B_2^X	9					1
E^X	17				1	1
A_1^L	14	1				1
A_2^L	10		1		1	
E^L	24			1	1	1
DIMS	576	8	8	16	24	24

Table 2. Irreducible representations of O corresponding to the representations induced in O by D_2'.

	$A_1\uparrow$	$B_1\uparrow$	$B_2\uparrow$	$B_3\uparrow$
A_1	1			
A_2		1		
E	1	1		
T_1		1	1	1
T_2	1		1	1
DIMS	6	6	6	6

3. Induced representations and Frobenius's reciprocity theorem

Frobenius (1903; Ledermann 1977, Altmann 1977) has given a general procedure for generating representations of the group G which are 'induced' by irreducible representations of an arbitrary subgroup $H \subset G$. We shall follow the exposition of

Ledermann (1977, p 69), omitting proofs but making some comments about the physical interpretation of the mathematics. We have already shown that the decomposition of G into $r = |G|/|H|$ left cosets has a direct significance in relation to the decomposition of a system into similar subsystems. We write

$$G = \bigcup_{i=1}^{r} g_i H \tag{3.1}$$

where the set of r operators $g_i \in G$ includes the identity.

Let $\boldsymbol{R}(x)$ $(x \in H)$ be an irreducible representation of H generated by an n-dimensional subsystem basis with the convention that $\boldsymbol{R}(x) = 0$ if $x \in G$, $x \notin H$. The $(r \times n)$-dimensional representation induced by H in G is defined as

$$\boldsymbol{S}(x) = [\boldsymbol{R}(g_i^{-1} \times g_j)] \tag{3.2}$$

where the matrix $\boldsymbol{S}$ contains r^2 submatrices $\boldsymbol{R}$. These submatrices are zero if $g_i^{-1} \times g_j \notin H$, and it can be shown that only one submatrix survives in any row or column. Hence $\boldsymbol{S}$ permutes complete subsystem bases but does not mix their components.

A simple formula can be derived which relates the characters of the representations χ_H of H to the characters χ_G of their induced representations in G. If $h(x)$ and $g(x)$ denote the numbers of elements in the classes containing x in H and G, respectively, we may write

$$\begin{aligned} \chi_G(x) &= r \sum \chi_H(x) h(x)/g(x) \qquad (x \in H) \\ &= 0 \qquad\qquad\qquad\qquad\quad (x \notin H) \end{aligned} \tag{3.3}$$

where the sum is taken over all classes in H that correspond to a specific class in G and $r = |G|/|H|$ is the same quantity as was introduced above. A trivial consequence of this formula is that the regular representation of H induces the regular representation of G.

Frobenius also proved the 'reciprocity theorem', which states that the number of times an irreducible representation Γ_α of G appears in the representation $\Gamma(\gamma_\beta)$ induced by the irreducible representation γ_β of H is equal to the number of times γ_β appears in a reduction of Γ_α with respect to H. This theorem has also been called the 'correlation theorem' by Wilson *et al* (1955) and Newman (1981). Its value is that it provides a means of using subgroups to provide as unique symmetry labelling of the states of a system rather than the more familiar method of using higher (essentially fictitious) symmetry groups. An example of this application can be found in Newman (1981) where it is employed to obtain a unique group-theoretical labelling of the displacements in shells of atoms in cubic crystals. The idea, which can be carried over to the general context of the present discussion, is to use subgroup irreducible representation labels to distinguish repeated occurrences of a given irreducible representation of G in the state space of the complete system. The circumstances in which this may be carried out are a trivial consequence of the reciprocity theorem.

If the reduction of the irreducible representations of G with respect to $H \subset G$ is unique (in the sense that no H representation is repeated in a given reduction), then uniquely labelled bases corresponding to the states of a subsystem of symmetry H may be used to provide unique labels for the induced bases of direct sum system of symmetry G. It should be noted that this result depends on the fact that the maximal basis under consideration corresponds to a regular representation of G.

The work of Newman (1981) shows explicitly how such a labelling is achieved for several possible subsystems of an O_h system. In particular, it is shown that C'_{2v} subsystems provide a unique labelling of the O_h normal nodes of vibration. This example points to the value of using subsystems whose symmetry properties can be described by an Abelian subgroup of the system group.

4. Direct products of induced representations

Ledermann (1977) and Altmann (1977) both discuss an interesting series of theorems due to Mackey (1951, 1952, 1953), which relate to the irreducible representations which appear in inner direct products of induced representations. The idea behind these theorems is to analyse the direct products into a sum of representations corresponding to the various possible relationships between subsystems. Remembering, from § 2, that the relationships between subsystems (and their corresponding subgroups) have structures related to the double coset analysis of the group, it comes as no great surprise to find that Mackey's final theorem expresses the inner direct product in terms of a sum over contributions labelled by double cosets. We shall again restrict consideration to double cosets generated by a single subgroup, so that the form of Mackey's theorem given below is a special case.

Let χ^i_α, χ^i_β denote the characters of two representations of the subgroup H_i of G. We shall write $(\chi^i_\alpha \uparrow G)$, $(\chi^i_\beta \uparrow G)$ for the characters of the corresponding representations induced in G. Following § 2 we write $\Delta_i = H_1 \cap H_i$. It can be shown (Ledermann 1977, page 86) that the products

$$\zeta_i(x) = \chi^i_\alpha(x)\chi^1_\beta(x) \qquad (x \in \Delta_i) \tag{4.1}$$

are characters of Δ_i, and that the induced characters satisfy the relation

$$(\chi^1_\alpha \uparrow G)(\chi^1_\beta \uparrow G) = \sum_{i=1}^{r} (\zeta_i \uparrow G) \tag{4.2}$$

for all operators in G. Altmann (1977, p 155) formulates this theorem more explicitly in terms of inner direct products of the induced representations. He also extends it (p 157) to the triple inner direct product of induced representations.

It is apparent that equation (4.2) analyses the product representation into components corresponding to each possible relationship between subsystems (enumerated by i). Provided that $(\zeta_i \uparrow G)$ gives a unique labelling of the representations of G, we see that the addition of the subsystem relationship label i should provide for a unique labelling of the direct product representations of G.

As a specific example of a labelling problem that can be solved by using Mackey's theorem we consider the representation produced by the direct product of O_hT_{1g} representations induced into $G = O_h^5/(2\text{FCC})$. This may be reduced with respect to G (forming an *inner* direct product) to give the following $24^2 = 576$-dimensional representation:

$$\begin{aligned} T_{1g}\uparrow \otimes T_{1g}\uparrow = {} & 5A^\Gamma_{1g} + 2A^\Gamma_{2g} + 7E^\Gamma_g + 8T^\Gamma_{1g} + 9T^\Gamma_{2g} + 12A^X_{1g} + 8A^X_{2g} + 9B^X_{1g} + 9B^X_{2g} \\ & + 17E^X_g + 14A^L_{1g} + 10A^L_{2g} + 24E^L_g. \end{aligned} \tag{4.3}$$

This equation may be obtained from table 1, or directly from the character table given by Chan and Newman (1982, table 5). In order to simplify the following discussion

we shall drop the labels g which indicate inversion symmetry and seek to analyse the above expression in terms of the chain

$$D_2' \subset O \subset G_P$$

where G_P is the 192-element group corresponding to the proper rotations and (two-fold cyclic) translations in G. Tables 1 and 2 give the correlations between irreducible representations for this chain, and show that it provides a unique labelling scheme in the sense of Newman (1981).

We are interested in possible ways of providing group-theoretical labels to distinguish repeated representations on the right-hand side of (4.3). One approach would be to expand $T_1\uparrow$ in terms of G_P representations (see table 1):

$$T_1\uparrow = T_1^{\Gamma} + A_2^{X} + E^{X} + A_2^{L} + E^{L}.$$

This allows us to analyse the right-hand side of (4.3) in terms of G_P representations but, as this group is not simply reducible (see Chan and Newman 1982, table 5) a unique labelling is not, thereby, obtained. However, the double coset decomposition does provide a way of obtaining a unique labelling scheme.

According to Mackey's theorem (equation (4.2)) the product representation $T_1\uparrow \otimes T_1\uparrow$ can be expressed as a sum over induced representations of direct product representations of the subsystem intersection groups D_2' and O (corresponding to the Δ_i in equation (4.1)). In the case of the intersection group O, the term on the right-hand side of (4.2) contributing to (4.3) is

$$\begin{aligned}(T_1 \otimes T_1)\uparrow &= A_1\uparrow + E\uparrow + T_1\uparrow + T_2\uparrow \\ &= A_1|A_1^{\Gamma} + A_1|A_1^{X} + A_1|A_1^{\Gamma} + E|E^{\Gamma} + E|A_1^{X} + E|B_1^{X} + E|E^{L} + T_1|T_1^{\Gamma} + T_1|A_2^{X} \\ &\quad + T_1|E^{X} + T_1|A_2^{L} + T_1|E^{L} + T_2|T_2^{\Gamma} + T_2|B_2^{X} + T_2|E^{X} + T_2|A_1^{L} + T_2|E^{L}. \quad (4.4)\end{aligned}$$

Here the second equality follows from table 1. The inducing representation label of the group O is retained (Newman 1981) to distinguish between repeated representations, such as the three occurrences of E^{L}.

Two 72-dimensional representations $(T_1 \otimes T_1)\uparrow$ occur, corresponding to the self-interaction of the subsystem (with double coset containing the elements of the group O) and the interaction of subsystems displaced by t'. Hence the labels E, t' must also be retained in order to distinguish these two sets of similar representations. The remaining part of expression (4.3) is produced by the representations induced in G_P by the representation of the interactions group D_2' using the correlations given in table 2. We obtain

$$\begin{aligned}T_1 \otimes T_1 \rightarrow (B_1 + B_2 + B_3) \otimes (B_1 + B_2 + B_3) \\ = (B_1 \otimes B_1)A_1 + (B_2 \otimes B_2)A_1 + (B_3 \otimes B_3)A_1 + (B_1 \otimes B_2)_e B_3 \\ + (B_1 \otimes B_2)_e B_3 + (B_2 \otimes B_3)_e B_1 \\ + (B_2 \otimes B_3)_o B_1 + (B_1 \otimes B_2)_o B_3 + (B_1 \otimes B_3)_o B_2. \quad (4.5)\end{aligned}$$

Here the direct product origin of each representation has to be retained for unique labelling. The subscripts e, o distinguish the even and odd part of direct products of distinct representations. Taking the first representation as an example, we find using

table 2 that it induces the following representation into O:

$$(B_1 \otimes B_1)A_1\uparrow = (B_1 \otimes B_1)A_1|A_1 + (B_1 \otimes B_1)A_1|E + (B_1 \otimes B_1)A_1|T_2$$
$$= B_1^2|A_1 + B_1^2|E + B_1^2|T_2.$$

In the last line we have removed redundant symbols, retaining only the B_1^2 which distinguishes this A_1 representation of D_2' from the other two. The next step is the further induction of this representation into G_P, giving

$$(B_1 \otimes B_1)A_1\uparrow\uparrow = B_1^2|A_1|A_1^\Gamma + B_1^2|A_1|A_1^X + B_1^2|A_1|A_1^L + B_1^2|E|E^\Gamma + B_1^2|E|A_1^X + B_1^2|E|B_1^X$$
$$+ B_1^2|E|E^L + B_1^2|T_2|T_2^\Gamma + B_1^2|T_2|B_2^X + B_1^2|T_2|E^X + B_1^2|T_2|A_1^L + B_1^2|T_2|E^L,$$

In this case it is necessary to retain both a D_2' and O label to ensure unique labelling of the G_P representations.

It will be apparent that the remaining eight expressions in equation (4.5) can be treated similarly, leading to unique group-theoretical labels for all the components in the expansion of $[(B_1 + B_2 + B_3) \otimes (B_1 + B_2 + B_3)]\uparrow\uparrow$. This $9 \times 6 \times 8 = 432$–dimensional representation, which should be distinguished by the label t corresponding to the translation between subsystems defined by Chan and Newman (1982, § 4), completes the expansion of $T_1\uparrow \otimes T_1\uparrow$ as required. Hence, every term in equation (4.3) can be provided with a unique label using Mackey's theorem (equation (4.2)). In general, we note that this depends on finding a chain of subgroups corresponding to the Δ_i, equation (4.1), which (*a*) provides a unique labelling scheme and (*b*) in which all the subgroups are simply reducible.

The procedure exemplified in this section is thus seen to provide an important extension to the concept of unique labelling. It allows the use of groups in unique labelling schemes which are not themselves simply reducible, provided that a suitable chain of simply reducible subgroups (covering the Δ_i) exists.

5. Subsystems with non-interacting components

The relationship between Wannier and Bloch functions has been formulated in group-theoretical terms by des Cloizeaux (1963), who exploited the fact that the Wannier functions induce representations of the space group. This procedure follows the standard method of describing space group irreducible representations (Altmann 1977 and references therein). des Cloizeaux (1963) also studied the relationship between molecular orbitals and localised states in small lattice systems, such as a tetrahedron of lattice points.

More recently Newman (1974a) has discussed the relationship between Bloch states on a lattice of symmetry G and Bloch states on a set of equivalent sublattices† of symmetry $H \subset G$. If an infinite lattice is considered, H and G can be chosen to be isomorphic, yet the subgroup relationship is preserved because all the translation operators in H are fixed integral multiples of those in G. The physical idea exploited in this formalism is that, provided the sublattice is sufficiently sparse, its Bloch states lose their dispersion in $\boldsymbol{k}$ space, the highly degenerate energy level being equivalent to that of a Wannier function defined on the original lattice. As a result, it is possible

† There is some confusion in the literature regarding the usage of the terms 'sublattice' and 'superlattice'. In this work a *sublattice* is invariant under the operations in a subgroup of the original lattice group.

to use band energies at relatively few points in the Brillouin zone to determine the energies and interaction energies of the Wannier functions. If the band energies are known for a sufficient number of $\boldsymbol{k}$ values, it is relatively easy to determine the accuracy of this procedure, which has been called the *decoupling transformation*.

A similar formalism relates phonon dispersion curves with localised atomic displacements (Newman 1974b). The difference in this case is that the dispersion curves have normally been determined experimentally.

In order to demonstrate the application of the decoupling transformation to finite systems, as well as infinite lattices, we shall employ a very simple example which is capable of interpretation in both ways. Figure 3 shows a system comprising four subsystems, numbered 1 to 4. Each subsystem comprises two (atomic) components labelled a, b, which we assume to be far enough apart to be non-interacting. For the purposes of discussion we associate each component with a single s state, so that the one-electron states of the complete system are described by an eight-element vector. Alternatively, we can regard figure 3 as being embedded in a simple cubic lattice, so that the state vectors have infinite dimensionality.

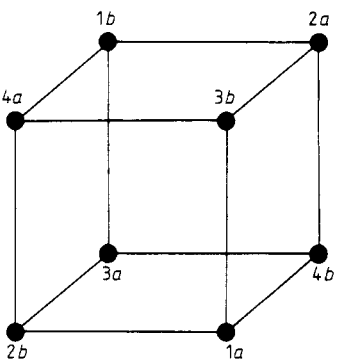

Figure 3. O_h system constructed from four equivalent non-localised subsystems numbered from 1 to 4.

If E_0 represents the energy of an isolated s state and E_1 is the interaction energy between nearest-neighbouring s states, the total energy matrix may be written as follows:

	$1a$	$1b$	$2a$	$2b$	$3a$	$3b$	$4a$	$4b$
$1a$	E_0			E_1		E_1		E_1
$1b$		E_0	E_1		E_1		E_1	
$2a$		E_1	E_0			E_1		E_1
$2b$	E_1			E_0	E_1		E_1	
$3a$		E_1		E_1	E_0			E_1
$3b$	E_1		E_1			E_0	E_1	
$4a$		E_1		E_1		E_1	E_0	
$4b$	E_1		E_1		E_1			E_0.

(5.1)

As the s states are invariant under inversion this operation can be omitted from our group-theoretical description. It is, therefore, sufficient to regard the complete system

as being invariant under the octahedral group O, and the subsystems 1 to 4 as being invariant under $D_3 \subset O$.

A partial diagonalisation of the matrix (5.1) can be achieved using the subsystem symmetry D_3. The pairs of s states for each subsystem may be combined to form a symmetric combination corresponding to the A_1 representation of D_3, or an antisymmetric combination corresponding to A_2. With this basis (5.1) becomes

$$\begin{array}{cc|cccc|cccc} & & \multicolumn{4}{c|}{A_1} & \multicolumn{4}{c}{A_2} \\ & & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \\ A_1 & 1 & E_0 & E_1 & E_1 & E_1 & & & & \\ & 2 & E_1 & E_0 & E_1 & E_1 & & & & \\ & 3 & E_1 & E_1 & E_0 & E_1 & & & & \\ & 4 & E_1 & E_1 & E_1 & E_0 & & & & \\ A_2 & 1 & & & & & E_0 & -E_1 & -E_1 & -E_1 \\ & 2 & & & & & -E_1 & E_0 & -E_1 & -E_1 \\ & 3 & & & & & -E_1 & -E_1 & E_0 & -E_1 \\ & 4 & & & & & -E_1 & -E_1 & -E_1 & E_0 \end{array} \tag{5.2}$$

The induced representations in O corresponding to A_1 and A_2 are given by

$$A_1\uparrow = A_1 + T_2 \qquad A_2\uparrow = A_2 + T_1.$$

The matrix (5.2) can be trivially diagonalised to give eigenvalues corresponding to each irreducible representation of O:

$$A_1\begin{cases} A_1\colon E_0+3E_1 \\ T_2\colon E_0-E_1 \end{cases} \qquad A_2\begin{cases} A_2\colon E_0-3E_1 \\ T_1\colon E_0+E_1 \end{cases}. \tag{5.3}$$

The difference of sign of E_1 in each pair of solutions is clearly associated with the relative phases of the component s states in the subsystems. In the case when the system of figure 3 is a simple cubic lattice (still with four subsystems) embedded in a simple cubic lattice, each of the four solutions can be associated with a different point in the corresponding Brillouin zone. Referring to table 1 of Newman (1974) for both energy expressions and notation we find the correspondence:

$$\begin{aligned} &A_1\colon \Gamma;\ \boldsymbol{k} = (000) && T_2\colon M;\ \boldsymbol{k} = (110), \text{ etc} \\ &T_1\colon X;\ \boldsymbol{k} = (100), \text{ etc} && A_2\colon R;\ \boldsymbol{k} = (111). \end{aligned} \tag{5.4}$$

Alternatively, we may embed the subsystems into a face-centred cubic system. Table 4 of Newman (1974) then allows us to set up a correspondence with a single pair of solutions

$$A_1\colon \Gamma;\ \boldsymbol{k} = (000) \qquad T_2\colon X;\ \boldsymbol{k} = (200), \text{etc.} \tag{5.5}$$

It is also necessary to note that in this case the interaction energy $I(\frac{11}{22}0) = \frac{1}{2}E_1$.

The form of the solutions (5.3) makes it clear that there is a simple relationship between two sets corresponding to different D_3 irreducible representations. The transformation $A_1 \rightarrow A_2$ is effected by a change in the relative sign of the component wavefunctions which, in turn, produces a change in sign of the interaction energy E_1. Hence, having obtained the solutions for *one* of the irreducible representations of the subgroup we can generate all the others simply by noting the effect on interaction energies. In the case of infinite lattice systems this enables us to obtain an expression

for the band energy at arbitrary points in $\boldsymbol{k}$ space. From this point of view all four solutions in (5.3) and (5.4) are given by the formula

$$E(\boldsymbol{k}) = E_0 + E_1(\cos \pi k_1 + \cos \pi k_2 + \cos \pi k_3) \tag{5.6}$$

which also interpolates the solutions at other points in $\boldsymbol{k}$ space.

In general, therefore, the method is to solve the problem in terms of interactions between subsystems and then to generalise the solutions to allow for possible phase differences between subsystem components. Finite systems will allow only a finite set of phase relations, whereas infinite lattices give rise to a continuum of solutions within the Brillouin zone.

6. Discussion

We have developed the physical interpretation of several mathematical results concerning the properties of induced representations. The emphasis has been on finding unique group-theoretical labels to describe the states of complex systems, on the basis that such descriptions provide an essential first step in the solution of dynamical problems.

A search of the literature has revealed several other different (and hitherto independent) strands of development related to the properties of induced representations. The work of Lulek (1980), Kuzma *et al* (1980) and Litvin (1982) has been centred on the analysis of physically determined representations into irreducible components. The methods used by Litvin (1982) are exactly analogous to those described by Newman (1981) and Chan and Newman (1982), although Litvin gives less explicit consideration of the problem of unique labelling.

There has also recently been considerable interest in the application of these techniques in the description of molecular symmetry, particularly in the case of non-rigid molecules, where a natural analysis into internally rigid subsystems may be useful. Work of this nature is described by Frame (1979).

Seligman (1979) discusses the application of double coset theory in the evaluation of matrix elements. This implicitly involves Mackey's theorem (see § 4) as the system matrix elements are decomposed into a sum involving the various possible inter- and intra-subsystem matrix elements.

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