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Point Symmetry Groups and Operators Revisited

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Abstract. We have studied finite point symmetry group (PSG) operators. Hermitian and unitary properties of these operators were deduced by analyzing their matrix representations. We showed that PSG operators: E, C_2, σ and S_2, and PSG groups: C_1, C_i, C_2, C_s, D_2, C_{2v}, C_{2h} and D_{2h} are the only unitary and hermitian ones. The algebraic relationships between point symmetry groups are analyzed on the basis of *isomorphism*, *homomorphism* and *descent-of-symmetry*. Hasse diagram for homomorphic PSG is derived for the first time.

1 Introduction

The hermitian and unitary operators, symmetry groups and their mutual relationships are fundamental to quantum mechanics and as such are invariably discussed in most standard or advanced textbooks [1]. However, some operator properties and group relationships are not always considered. For example, unitary properties of symmetry operators are usually mentioned within the context of continuous rotation groups and Lie groups, but rarely in the context of finite symmetry groups.

Likewise, while the *isomorphism* and group-subgroup (*descent-of-symmetry*) relationships are often discussed, other relationships between PSGs (e.g. *homomorphism*) have not been studied. The *descent-of-symmetry* is a transformation which converts a group (sometimes called parent group) into one of its subgroups.

Our aim is to complement these studies by extending the discussion of unitary and hermitian operators to finite groups and by examining *homomorphism* amongst the PSG.

2 Results and Discussion

A. Hermitian and unitary properties

Point symmetry groups contain the following elements (operators): E, C_n, S_n σ, (where S_n= σ x C_n). We shall start our analysis by deriving unitary and hermitian properties of these operators on the basis of their matrix representations.

E is obviously hermitian and unitary since its representation matrix is a unit matrix.

The explicit properties and forms for other operators can be obtained by noting that (in general) a unitary matrix u can always be expressed in the form $u=e^{iH}$ where H is a hermitian matrix. Since for unitary matrices $u=u^t$, $e^{2iH}=I$, where I is the unit matrix. The general form of H can then be readily derived.

In order to determine which C_n operators are hermitian and unitary we can utilize the eigenvalues calculated for general 3-dimensional rotation matrix [2]. The eigenvalues are 1, $e^{\pm i\Theta}$ where Θ is the rotation angle equal to $2\pi/n$. The standard relationship (1)

$$e^{\pm i\Theta} = (\cos\Theta \pm i\sin\Theta) \qquad (1)$$

then indicates that only for n=1,2 will all eigenvalues be real. The magnitude of eigenvalues for C_1 and C_2 will be unity. Thus one can conclude that only $C_1 \equiv E$ and C_2 operators are hermitian, because such operators must have all real eigenvalues. These operators are also unitary because their eigenvalues have absolute value of unity.

Hermiticity and unitarity of symmetry plane (σ) operator can be analyzed in a similar way by considering its representation matrix. If one chooses a general point P(x, y, z) and an arbitrary symmetry plane described by the equation $\alpha x+\beta y+\gamma z=0$ (which for point symmetry groups must pass through the origin), the transformation matrix deduced from solid geometry relationships [3] becomes:

$$\sigma = \begin{matrix} 1-2\alpha^2 & -2\alpha\beta & -2\alpha\gamma \\ -2\alpha\beta & 1-2\beta^2 & -2\beta\gamma \\ -2\alpha\gamma & -2\beta\gamma & 1-2\gamma^2 \end{matrix} \quad (2)$$

where α, β, γ are direction cosines of the plane normal. (2) has the eigenvalues:

$\varepsilon_1 = 1$, $\varepsilon_2 = 1$, $\varepsilon_3 = 1-2\gamma^2-2\beta^2-2\alpha^2$

which are real and have absolute value of unity (N.B. $\alpha^2+\beta^2+\gamma^2=1$). This proves σ operator to be hermitian and unitary.

S_n operators are defined as $S_n \equiv \sigma \times C_n$ i.e. a C_n rotation followed by reflection.

The eigenvalues (ε_i) of the product matrix $\sigma \times C_n$ are:

$$\varepsilon_1= \alpha^2-2\alpha^4+\beta^2-4\alpha^2\beta^2-2\beta^4+\cos(2\pi/n)-3\alpha^2\cos(2\pi/n)+2\alpha^4 \cos(2\pi/n)-3\beta^2 \cos(2\pi/n)+$$
$$+4\alpha^2\beta^2 \cos(2\pi/n)+2\beta^4 \cos(2\pi/n)+\gamma^2-4\alpha^2\gamma^2-4\beta^2\gamma^2-3\gamma^2 \cos(2\pi/n)+4\alpha^2\gamma^2 \cos(2\pi/n)+$$
$$+4\beta^2\gamma^2 \cos(2\pi/n)-2\gamma^4+2\gamma^4 \cos(2\pi/n)$$

$$\varepsilon_2= \cos(2\pi/n) + [-\alpha^2\sin^2(2\pi/n) -\gamma^2\sin^2(2\pi/n) - \beta^2\sin^2(2\pi/n)]^{1/2}$$
$$\varepsilon_3= \cos(2\pi/n) - [-\alpha^2\sin^2(2\pi/n) -\gamma^2\sin^2(2\pi/n) - \beta^2\sin^2(2\pi/n)]^{1/2}$$

Incidentally, the matrices of both products $\sigma \times C_n$ and $C_n \times \sigma$ have the same eigenvalues which indicates that σ and C_n operators commute for any integer value of n.

These eigenvalues are real (and unity) if and only if n=1,2 and hence the only hermitian and unitary S_n operator is $S_2 \equiv i$.

Hermitian (unitary) groups are those whose elements are hermitian (unitary) operators.

Inspection of PSG tables [6] shows that only groups C_1, C_i, C_2, C_s, D_2, C_{2v}, C_{2h} and D_{2h} are hermitian and unitary.

Hermitian groups are Abelian. This assertion follows from the rule that the product of two Hermitian operators is Hermitian if and only if the two operators commute [4] . The group property requires that the product of any two elements in the hermitian group is also hermitian, therefore the elements must commute and the group must be Abelian. The physical significance of hermitian group is that it represent a collection of observable properties which can be simultaneously determined with infinite accuracy.

B. Homomorphism

The three relationships of *isomorphism* , *homomorphism* and *descent-of-symmetry* are often mentioned in the context of applied group theory. *Descent-of-symmetry* and *isomorphism* are used in the symmetry analysis of many physical problems and all PSGs have been classified according to these group theoretical concepts [6,7]. The *descent-of-symmetry* finds mathematical expression in the notion of group-subgroup relationship and is presented through subgroup decomposition patterns [6]. All three relationships are transitive [8] i.e. if $A \supset B$ and $B \supset C$ then $A \supset C$. However, only *isomorphism* is symmetric i.e. if $A \cong B$ than $B \cong A$. Transitivity is useful in designing tables and graphs summarizing these properties because it reduces clutter, by allowing some lines connecting groups to be omitted.

In Fig.1 we present for the first time, a graph showing homomorphic relationships between point symmetry groups. The line between two groups indicates a parent group (which must be of higher order) and it's homomorphic image (lower order). A comparison between Fig.1 and graphs in ref. 6 shows that *descent-of-symmetry* and *homomorphism* are totally different properties, because the homomorphic image need not be a subgroup of the parent group. One must emphasize that although the *descent-of-symmetry* and *homomorphism* are both represented by *Haase* type diagrams, there is an important difference between the two properties. A line in the diagram related to *descent-of-symmetry* connects group (G) with its subgroup. In *homomorphism* the line connects the group (G) and its (homomorphic) image, which is not necessarily a subgroup of G. For example, C_3 is a subgroup of D_3, but not an image of it because there is no invariant subgroup H of D_3 for which it would apply that $D_3/H \cong C_3$. Thus in *descent-of-symmetry* diagram there would exist a line connecting D_3 and C_3, while no such line is present in Fig.1. The Fig.1 can be obtained by first deducing all possible invariant subgroups of each

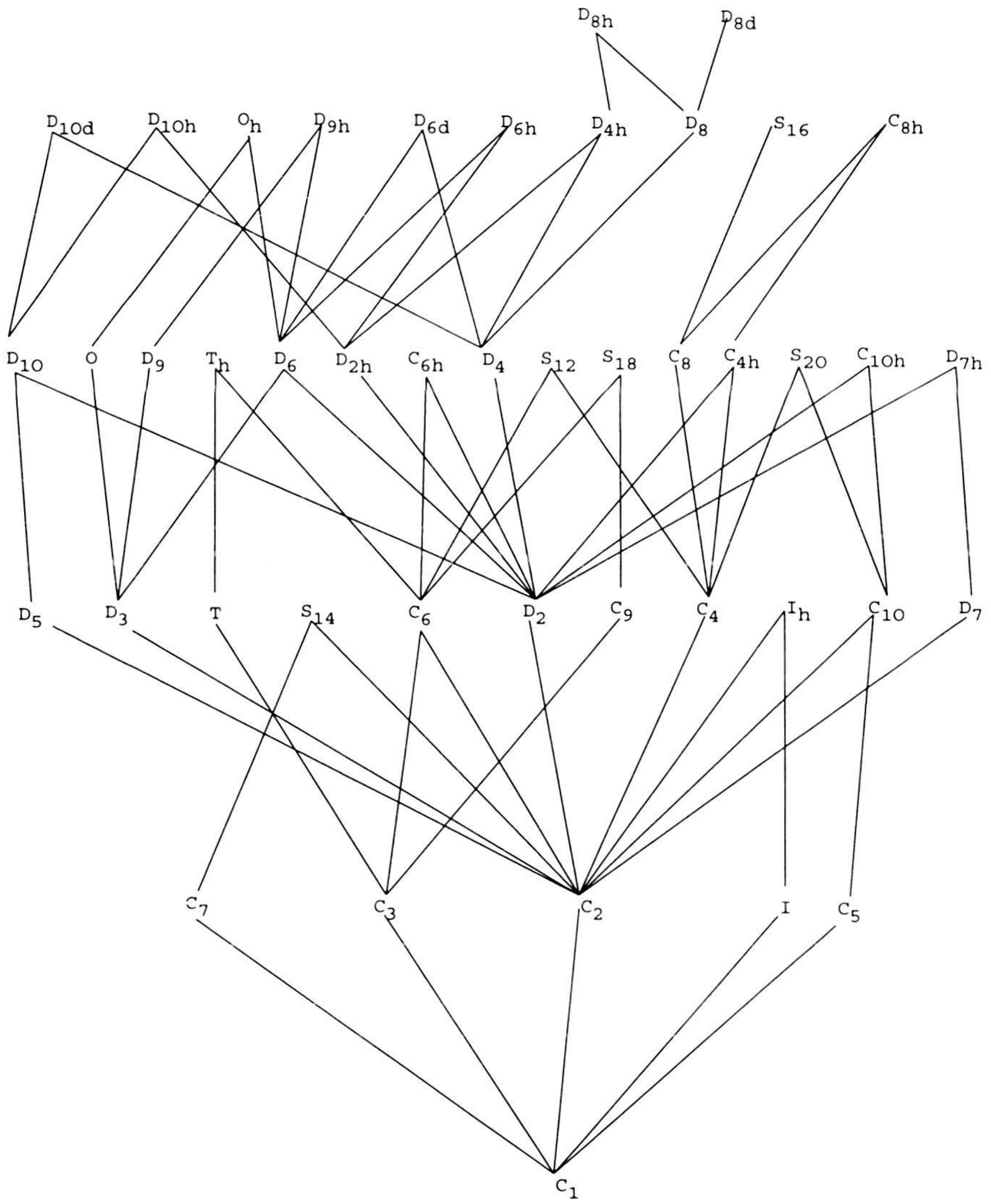

Figure 1

Molecular homomorphisms (Hasse diagram). The *homorphic* images are shown for all important point symmetry groups. Since *isomorphic* PSG have the same images, only one member of each *isomorphic* set is given in the graph.

point group and then assembling them in decreasing order using transitivity property. The groups of highest order which also have the largest number of invariant subgroups are then placed on top of the diagram. One can work its way down the diagram by considering groups of steadily decreasing order. Extension of a group is pertinent to our analysis of *homomorphism.* Consider any two groups G_1 and G_2 connected by the line on the diagram (and assuming $|G_1| > |G_2|$). Also assume that $K \subseteq G$, i.e. K being a certain invariant subgroup of G. Then, G_1 represents an extension of K by G_2.

C. Physical significance

In quantum mechanics the probability is given by the square of the state function and the state-to-state transition probability by the scalar product of state functions. These products are, of course, invariant under symmetry transformations. The set of transformations which satisfy this condition is unitary group. The important question is how are these symmetry relationships related to observable properties? For example, isomorphic molecules are considered to be equally symmetrical and yet their properties differ widely. Molecules of C_2 symmetry are chiral while those of isomorphic symmetries C_s and C_i are not; molecules of C_{nv} symmetry are polar while the isomorphic D_n are not. The different physical properties of isomorphic molecules can be related to the fact that the quantum mechanical operator which describes a certain physical property Π must commute with every symmetry operator (element) Σ_i in the point symmetry group (PSG) if it's expectation value is to be non-zero. In mathematical language: only if

$$[\Pi , \Sigma_i] = 0 \text{ for every i then } \langle\Pi\rangle \neq 0 \text{ typically} \qquad (3)$$

[Two assumptions are relevant here; the expectation is with respect to a symmetry-adapted state of a 1-dimensional irreducible representation and molecular property is an expectation over scalar (not vector or tensor) property].

The condition (3) is not fulfilled for some isomorphic groups and hence the molecular properties differ. The *isomorphism* is an abstract mathematical concept which considers only intra-group relationships (between group elements) and not the types of symmetry elements. *Homomorphism* also, does not bear a direct relationship to observable properties because it is based on the intra-group relationship, disregarding the nature of symmetry elements (operators).

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