Lecture Notes In Group Theory

17 maj 2007

Definition 1 (Group)**.** A set $\{a, b, \ldots\}$ form a *group* $\mathcal{G}$ if

1. There exists an composition law
$$a \cdot b = ab$$
that is associative, i.e.
$$(ab)c = a(bc).$$

2. The set is closed under this law, i.e.
$$ab = c \in \mathcal{G}; \qquad \forall a, b \in \mathcal{G}.$$

3. There exists an element $e \in \mathcal{G}$ with the property
$$ea = a \qquad \forall a \in \mathcal{G}$$
which we call the identity.

4. Every element $a \in \mathcal{G}$ has an inverse, denoted $a^{-1} \in \mathcal{G}$ defined by
$$aa^{-1} = e.$$

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Remark that the composition law does not need to be commutative, i.e.

$$ab \neq ba$$

in general. A group that do have a commutative composition law are called an **Abelian** group. The definition for a continous group is the same, but we will not study continous groups until later. It should also be noted that ab is a unique element in $\mathcal{G}$. We see this by looking at $ab = ad$, if this where true, we can use the composition law and act with the inverse of a, a^{-1} from the left on both sides and we find that $a^{-1}ab = eb = b = d = ed = a^{-1}ad$.

Definition 2 (Subgroup)**.** A *subgroup* $\mathcal{H}$ of a group $\mathcal{G}$ is a subset that itself forms a group.

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Two subgruops that also exists are $\{e\}$ and $\mathcal{G}$ itself, these are called the **trivial subgroups**. Every other subgrup is called a **proper subgroup**.

Definition 3 (Order)**.** The *order* of a group $\mathcal{G}$ is the number of elements in $\mathcal{G}$, denoted

$$g = \text{ord}\,(\mathcal{G}).$$

$\blacksquare$

Groups of infinite order can be both infinetly countable or uncountable (including the continous groups).

Example 1. Group of the triangle

The equilateral triangle have three mirror symmetries, mirror-planes through the middle of a side and its opposite vetex, and three rotational symmetries, 0, $\frac{2}{3}\pi$ and $\frac{4}{3}\pi$. These symmetries form the group C_{3v}.

If we consider the ammonia molecule (NH_3), which looks like this triangle with hydrogen in its vertecies, and nitrogen elevated in the center. The ammonia molecule is however not symmetric with rotation π (when we 'flip' the molecule over) because of the nitrogen. So the group of the ammonia molecule is actually D_3.

We can represent the rotational symmetries by

$$\begin{aligned} e(a,b,c) &= (a,b,c) && (0 \text{ - rotation}) \\ c_3(a,b,c) &= (c,a,b) && (\frac{2}{3}\pi \text{ - rotation}) \\ c_3^2(a,b,c) &= (b,c,a) && (\frac{4}{3}\pi \text{ - rotation}). \end{aligned}$$

And the morror symmetries by

$$\begin{aligned} \sigma_a(a,b,c) &= (a,c,b) \\ \sigma_b(a,b,c) &= (c,b,a) \\ \sigma_c(a,b,c) &= (b,a,c). \end{aligned}$$

This notation σ_a is somewhat devious, it doesn't morror on the vertex a but rather on the first element of the sequence (i,j,k). It should also be kept in mind that the labeling of the vertecies are an abstract labeling. If we did label the the vertecies we would destroy the symmetries, since vertex a is different from vetex b etc. Also note ord $(C_{3v}) = 6$.

To prove that C_{3v} is a group, we will construct its **Composition table**, a table where we have preformed all pair compositions.

$\cdot$	e	c_3	c_3^2	σ_a	σ_b	σ_c
e	e	c_3	c_3^2	σ_a	σ_b	σ_c
c_3	c_3	c_3^2	e	σ_c		
c_3^2	c_3^2	e	c_3			
σ_a	σ_a	σ_b		e		
σ_b	σ_b				e	
σ_c	σ_c					e

Remark that every element of C_{3v} is in every row and in every collumn (sodoku), that proves that every element of C_{3v} has an inverse, since the identity is in very row/collumn. We also see that the group is non-Abelian.

We have two proper subgroups of C_{3v}

$$\begin{aligned} C_3 &= \{e, c_3, c_3^2\}, \\ C_S &= \{e, \sigma_a\} \cong \{e, \sigma_b\} \cong \{e, \sigma_c\}. \end{aligned}$$

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Just as we had in the example above, all groups have a composition table where all rows and collumns possess each element.

Example 2. Integers

The integers $\mathbb{Z}$ under addition forms an Abelian infinite descrete group.

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Example 3. Rotations in two dimensions

Rotations in two dimensions forms an Abelian continous group, where the angle addition is addition under modulus 2π. This group is called $SO(2)$.

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Example 4. Permutation of three identical particles

We have three positions labeled 1,2 and 3. We now represent the symmetry operations as a sequence of numbers, e.g. $(1, 2, 3)$. For example (1,2,3) means that particle in space 1 goes to 2, and the particle in 2 goes to 3 and the particle in 3 goes where there is space left, that is 1. The permutaion of three identical particles has several symmetry operations

$$\begin{gathered} (1,2,3), (1,3,2) \\ (1,2),\ (2,3),\ (3,1) \\ (1) \end{gathered}$$

In a mathematical sence, this is exactly the same group as C_{3v} (isomorphic to), but it is called P_3.

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Definition 4 (Mapping of a group)**.** If we can construct a map between two groups, from $\mathcal{G}$ to $\mathcal{H}$, we call it a

- *homomorphism* if $f(a)f(b) = f(ab)$, where we at the lefthand-side uses the composition law in $\mathcal{H}$ and the righthand-side uses the composition law in $\mathcal{G}$. One might call a homomorphism a mapping where "the composition is kept". We say in this case that $\mathcal{G}$ is *homomorphic* to $\mathcal{H}$, and denote it $\mathcal{G} \simeq \mathcal{H}$.

- *isomorphism* if it is a bijective (one-to-one) homomorphism. We then say that $\mathcal{G}$ is *isomorphic* to $\mathcal{H}$, and denote it $\mathcal{G} \cong \mathcal{H}$.

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Generators of a group

Definition 5 (Generators)**.** A groups *generators* is the smallest set of a group elements whose succesive composition generated the whole group.

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Example 5. G_6

Let's define a group by introducing two generators p, q and the following multiplication rules

$$p^3 = e, \quad q^2 = e, \quad (qp)^2 = e.$$

We then construct the group by looking at powers of the generators to begin with, i.e.

$$p,\ p^2,\ q.$$

must be elements in the group, but no higher powers, since that gives identity. The last multiplication rule indicates that qp also is an element of the group. We can then create one more element, qp^2 through combinations of the already existing elements. So we have the group

$$G_6 = \{e, p, p^2, q, qp, qp^2\}$$

which is the whole group. This might be hard to see, for example why isn't pqp an element of the group? This is since

$$pqpq = (pq)^2 = e \Rightarrow pqp = q^{-1} = q \text{ since } q^2 = e.$$

Remark here that

$$G_6 \cong C_{3v}$$

if we let $p = c_3$ and $q = \sigma_i$.

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We call a group G_n **cyclic** if G_n is defined by $p^n = e$, where p is G_n's only generator. In this case we call n the **order** of the gerator which allways is the same as the order of the group. Remark that $G_3 \cong C_3$.

Example 6. Integers

$\mathbb{Z}_n$ is a cyclic group, under addition, of order n, with $p = 1$ and $p^2 = 1 + 1$.

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Definition 6 (Cosets)**.** The *left coset* of a subgroup $\mathcal{H}$ of $\mathcal{G}$, devides $\mathcal{G}$ into disjoint subsets;

$$\mathcal{G} = \bigcup_{i=1}^{\operatorname{ord}\mathcal{G}} a_i\mathcal{H}; \quad a_i \in \mathcal{G}$$

where we have $b\mathcal{H} = \mathcal{H}$ if $b \in \mathcal{H}$ (because of the suduko-rule").

The *right coset* is instead defined by

$$\mathcal{G} = \bigcup_{i=1}^{\operatorname{ord}\mathcal{G}} \mathcal{H}a_i; \quad a_i \in \mathcal{G}.$$

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The number of cosets is

$$n = \frac{\operatorname{ord}\mathcal{G}}{\operatorname{ord}\mathcal{H}}.$$

Example 7. Cosets of C_{3v}

Let's study C_{3v} and it's subgroup C_3. The left coset representation of C_{3v} is then

$$C_{3v} = \{e, c_3, c_3^2\} \cup \{\sigma_a, \sigma_b, \sigma_c\}.$$

Notice that the first set is the subgroup C_3 and the other is a set generated by one of the $\sigma_i C_3$ unions. The right and the left coset of C_{3v} with respect to C_3 are the same. If we instead study C_{3v} with respect to the subgroup C_S we have the following left coset representaion

$$C_{3v} = \{e, \sigma_a\} \cup \{c_3, \sigma_c\} \cup \{c_3^2, \sigma_b\} = eC_S \cup c_3C_S \cup c_3^2C_S.$$

and the right coset is different

$$C_{3v} = \{e, \sigma_a\} \cup \{c_3, \sigma_b\} \cup \{c_3^2, \sigma_c\}.$$

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All cosets have the same number of elements. In the above example we see that we had three elements in every coset, with respect to C_3 and two elements in every coset with respect to C_S.

If the left and right coset are identical, then we say that $\mathcal{H}$ is a **normal** coset of $\mathcal{G}$. A group is called **simple** if it has *no* proper normal subgroups, and **semi-simple** if it has *no* proper Abelian normal subgroups. So from our examples we know that C_{3v} is neither simple nor semi-simple, since it do have an Abelian subgroup.

Definition 7 (Factor group)**.** The factor group of $\mathcal{G}$ and $\mathcal{H}$, denoted $\mathcal{G}/\mathcal{H}$, is a group where the elements are the cosets.

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Example 8. Factor group

$$C_{3v}/C_3 = \{eC_3, \sigma_a C_3\} \cong C_S$$

Even though the factor group is a group of sets, is can still be isomorphic to a group of just elements, since the do satisfy the same properties

$$eC_3\sigma_a C_3 = e\sigma_a C_3 C_3 = \sigma_a C_3.$$

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Combinations of groups

Definition 8 (Outer direct group)**.** A group $\mathcal{G}$ is called an *outer direct group* if it can be written as

$$\mathcal{G} = \mathcal{G}_1 \times \mathcal{G}_2$$

where the sets $\mathcal{G}_1$ and $\mathcal{G}_2$ has the following properties

- $\mathcal{G}_1 \subset \mathcal{G}$ and $\mathcal{G}_2 \subset \mathcal{G}$ where $\mathcal{G}_1 \cap \mathcal{G}_2 = \{e\}$.
- $\forall a_i \in \mathcal{G}_1$ and $\forall b_i \in \mathcal{G}_2$: $a_i b_j = b_j a_i \in \mathcal{G}$.

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The outer direct product '$\times$' is symmetric, i.e. $\mathcal{G} = \mathcal{G}_1 \times \mathcal{G}_2 = \mathcal{G}_2 \times \mathcal{G}_1$. And because of the second property of the subgroups must both be normal.

This could represent a object with both geometric symmetries, in $\mathcal{G}_1$ and some more abstract or internal symmetries, in $\mathcal{G}_2$, such as spin.

Example 9. Outer direct group
Consider the two groups

$$S_1 = \{e, i\}$$
$$C_2 = \{e, c_2\}$$

where the element i represents inversion, e.g. $r \longrightarrow -r$, mirroring in one point, and c_2 are rotation by π. We can then form the Outer direct group

$$\mathcal{G} = S_1 \times C_2 \cong S_2 = \{e, c_2, i, \sigma\}$$

with $\sigma = ic_2$.

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Definition 9 (Inner direct group)**.** A group $\mathcal{G}$ is called an *inner direct group* if it can be written as

$$\mathcal{G} = \mathcal{G}_1 \otimes \mathcal{G}_1 \cong \mathcal{G}_1$$

with elements $a_i a_j \in \mathcal{G}$ when $a_k \in \mathcal{G}_1$. Here what we mean by $a_i a_j$ is that a_i is in the "first" group $\mathcal{G}_1$ and a_j in the "second".

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This could represent a system of many particles that posesses the same symmetries.

Definition 10 (Semi-direct group)**.** Let $\mathcal{G}_1$ be normal to $\mathcal{G}$ and $\mathcal{G}_2$ not necessarily normal to $\mathcal{G}$. If these satisfies

- $\mathcal{G}_1 \cap \mathcal{G}_2 = \{e\}$,
- $a_i \in \mathcal{G}_1$, $b_j \in \mathcal{G}_2$ then $a_i b_j \in \mathcal{G}$,

We call *mathcalG* a semi-direct group, and denote this by

$$\mathcal{G} = \mathcal{G}_1 \wedge \mathcal{G}_2.$$

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Example 10. Semi-direct group
$C_{3v} = C_3 \wedge C_S$.

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Definition 11 (Conjugate classes)**.** If we for elements $a, b, t \in \mathcal{G}$ can write

$$b = tat^{-1}$$

we call b *conjugate* of a with respect to t. Let t be any element of $\mathcal{G}$, then the set $\{b\}$ produced by this conjugation is called the *class* of a.

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The conjugation of the elements $a \in \mathcal{G}$ lead to disjoint classes.

Example 11. Classes of C_{3v}
C_{3v} has three classes

$$K_1 = \{e\},\ K_2 = \{c_3, c_3^2\},\ K_3 = \{\sigma_a, \sigma_b, \sigma_c\}.$$

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The identity e allways form it's own class, infact a class is never a group, except $\{e\}$.

The dimension of a class, i.e. the number of elements, $r_a = \dim K_a$ is always a devisor of $\operatorname{ord} \mathcal{G} = g$, and $g = \sum_a r_a$. But the number of classes are not in general a devisor of the order of the group.

A normal subgroup $\mathcal{H}$ of $\mathcal{G}$ is a union of classes of $\mathcal{G}$.

Example 12. We see that $C_3 = K_1 \cup K_2$, but we cannot write C_S as a union of classes, and it is therefore not normal to C_{3v}.

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Representations

Definition 12 (Representation)**.** A *representaion* of a group $\mathcal{G}$ is a homomorphic map of the elements, $a \in \mathcal{G}$, on to a set of linear operators $D(a)$, acting in some vector space $\mathcal{L}$.

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What we will come to call the **dimension** of a representaion is just the dimesntion of the vector space (or even Hilbertspace) upon where the operators act.

Definition 13 (Matrix representation)**.** With a basis $\{|\, i\,\rangle\}$ spanning $\mathcal{L}$, we can define the *matrix representaion* of a operator $D(a)$ as

$$D_{ij}(a) := \langle\, i \mid D(a) \mid j\,\rangle\,.$$

This is the represetation we will encounter most in these lectures.

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Definition 14 (Identical representations)**.** Two representations, D' and D, are said to be *identical* if they are connected by a non-singular transformation S of the basis

$$\begin{aligned} &|\, i'\,\rangle = S|\, i\,\rangle \\ &D'(a) = S^{-1} D(a) S; \quad a \in \mathcal{G}. \end{aligned}$$

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Note the recemblence with ordinary basis change in linear algebra.

Among all mutaual identical representations there is allways one representation that is unitary, i.e. $D^{-1}(a) = D'^{\dagger}(a)$.

If we would take the trace of any representation of some element $\operatorname{Tr} D'(a)$ we see that

$$\operatorname{Tr} D'(a) = \operatorname{Tr}\left(S^{-1}D(a)S\right) = \operatorname{Tr}\left(SS^{-1}D(a)\right) = \operatorname{Tr} D(a).$$

This means that the trace is basis independent, so we can form some concept that is the same for all identical representations.

Definition 15 (Character)**.** The *character* of a representation is defined as the trace, denoted

$$\chi(a) = \operatorname{Tr} D(a).$$

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Let a and b be in the same class of some group $\mathcal{G}$, i.e. $a = tbt^{-1}$ with $t \in \mathcal{G}$. Then by studying the character of a and b in some representation we see that

$$\chi(b) = \chi(tat^{-1}) = \operatorname{Tr}\left(D(t)D(a)D(t^{-}1)\right) = \operatorname{Tr}\left(D(t^{-1})D(t)D(a)\right) = \operatorname{Tr}\left(D(e)D(a)\right) = \operatorname{Tr} D(a) = \chi(a)$$

since the composition law of the elements of the groups should hold in the representation. We see that for class elements the character is the same.

Definition 16 (Reducible representations)**.** A representation is said to be *reducible* if the Hilbertspace $\mathcal{L}$ posesses a non-trivial subspace $\mathcal{L}' \subset \mathcal{L}$, which is mapped onto itself by all operators $D(a)$ where $a \in \mathcal{G}$.

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If a representation is not reducible we say it is **irriducible**.

In general $\mathcal{L}$ can be decomposed in a direct sum of invariant subspaces, i.e. closed under action of its operators,

$$\mathcal{L} = \bigoplus_{\alpha} \mathcal{L}^{(\alpha)}$$

where the representations are irreducible in each subspace $\mathcal{L}^{(\alpha)}$

$$D(\mathcal{G}) = \bigoplus_{\alpha} D^{(\alpha)}(\mathcal{G}).$$

So if we would have a representation $D(\mathcal{G})$ of the same dimension as the Hilbertspace $\mathcal{L}$ we can by a non-singular transformation S transform $D(\mathcal{G})$ to $D'(\mathcal{G})$ where each element can be written as

$$D'(a) = \begin{bmatrix} D^{(1)}(a) & 0 & \dots & 0 \\ 0 & D^{(2)}(a) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & D^{(n)}(a) \end{bmatrix}$$

where $n \leq \dim \mathcal{L}$ and all $D^{(i)}(a)$ irreducible. And all elements have the same form since if it wouldn't, then for some $D^{(i)}(b)$ it wouldn't be in its irreducible form. More formally we write this as

$$D(\mathcal{G}) = \bigoplus_{\alpha}^{\text{inequiv}} m_\alpha D^{(\alpha)}(\mathcal{G})$$

where m_α is called the **multiplicity**, and counts the number of identical representations.

Example 13. "Triangular functions"-representation of C_{3v}

Here we will use a Hilbertspace spanned by the functions $\{f_1(\underline{x}), f_2(\underline{x}), f_3(\underline{x})\}$, where $f_i : \mathbb{R}^2 \longrightarrow \mathbb{R}$ are defined by

$$f_i(\underline{x}) = e^{-(\underline{x}-x_i)^2}$$

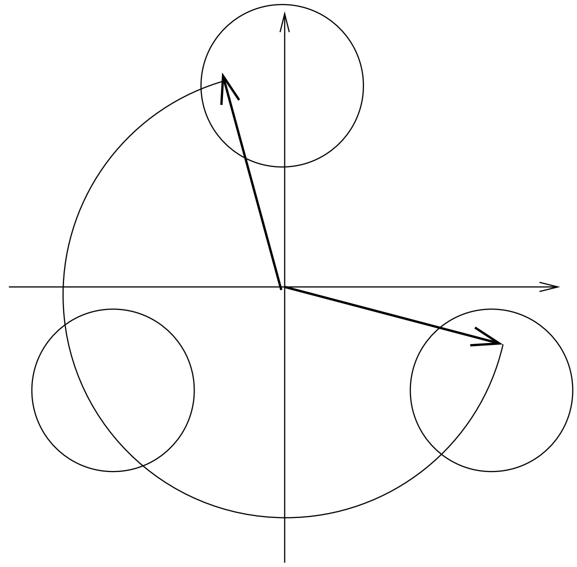
where x_i are the position of the i'th corner of the triangle. The functions only dependent on the distance from one of the corners x_i to the position $\underline{x}$. Since we have chosen a three dimenstional Hilbertspace we should also obtain a three dimensional representation of C_{3v}. The action of $D(a)$, $a \in \mathcal{G}$, upon a function is defined as

$$D(a) f_i(\underline{x}) := f_i(a^{-1}\underline{x})$$

where a^{-1} is taken as the faithful representaion.

If we let $D(c_3)$ act on, say, f_1

$$D(c_3) f_1(\underline{x}) = f_1(c_3^{-1}\underline{x}) = f_1(c_3^2\underline{x})$$



Since the functions are only distance dependent, we see from the picture above that

$$f_1(c_3^2\underline{x}) = f_2(\underline{x})$$

which is easily generalized to

$$D(c_3)f_i(\underline{x}) = \sum_{j=1}^{3} D_{ji}(c_3)f_j(\underline{x}).$$

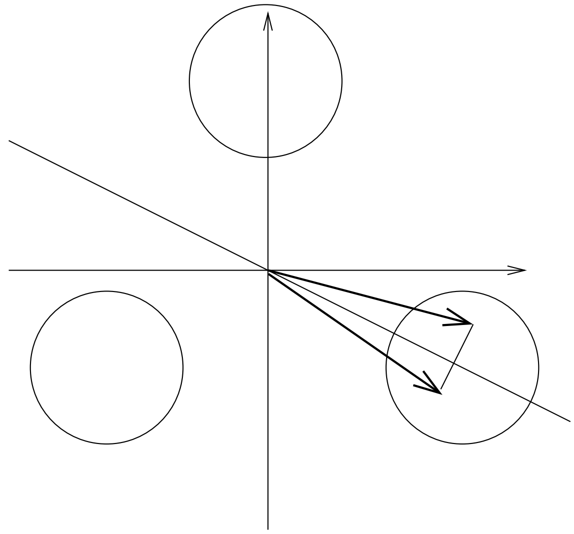
This provides us with the matrix corresponding to $D(c_3)$

$$D(c_3) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

with zero trace, so $\chi(c_3) = 0$. The matrix can be read in an easy way. Let the collumns represent the original function, i.e. first collumn corresponds to the first function, after action with the operator is where the 1 enters. So we read the matrix as first function goes to the second, the second function goes to the third and the third where it is space left, i.e. to the first.
The opposite direction, c_3^2 is just the transpose of this matrix

$$D(c_3^2) = D(c_3)^T = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

which also has zero trace $\chi(c_3^2) = 0$, since they are in the same class.



From the picture above we can also find the $D(\sigma_1)$ matrix. we see that $f_1 \longrightarrow f_1$, $f_2 \longrightarrow f_3$ and $f_3 \longrightarrow f_2$ so the matrix is

$$D(\sigma_1) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

This has the character $\chi(\sigma_1) = 1$. The other mirroring operators' representations can be found the same way. The identity is just the identity matrix

$$D(e) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

This has the character $\chi(e) = \dim \mathcal{L} = 3$.

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Example 14. The irreducible representations of C_{3v}

It is possible to show that

$$S = \begin{bmatrix} 1 & 0 & -2 \\ 1 & \sqrt{3} & 1 \\ 1 & -\sqrt{3} & 1 \end{bmatrix}$$

reduces the tree dimensional representation we just found into one one dimensional and one two dimensional irreducible representation. So for example we have

$$
\begin{aligned}
D'(c_3) &= S^{-1}D(c_3)S = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix} = \begin{bmatrix} D^{(1)}(c_3) & 0 \\ 0 & D^{(2)}(c_3) \end{bmatrix} \\
D'(\sigma_1) &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\end{aligned}
$$

And the corresponding characters

$$
\begin{aligned}
\chi(c_3) = 0, \quad \chi^{(1)}(c_3) = 1, \quad \chi^{(2)}(c_3) = -1, \\
\chi(\sigma_1) = 1, \quad \chi^{(1)}(\sigma_1) = 1, \quad \chi^{(2)}(\sigma_1) = 0.
\end{aligned}
$$

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The fundamental orthogonality relation for an irreducible representation

Theorem 1. For two irreducible representations, denoted α and β, of a group $\mathcal{G}$, with $\operatorname{ord}\mathcal{G} = g$, we have the following for a $b \in \mathcal{G}$:

$$
\sum_{a\in\mathcal{G}} D^{(\alpha)}_{ij}(a) D^{(\beta)}_{kl}(ba^{-1}) = \frac{g}{d_\alpha}\delta_{\alpha\beta}\delta_{ij}D^{(\alpha)}_{kj}(b) \tag{1}
$$

where $d_\alpha = \dim\alpha$.

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This is called a ortogonality relation since on the lefthand side of (1) contains $\delta_{\alpha\beta}$, which nonzero only when α and β are the same representation.

There is a special case of this relation, when $b = e$, the identity

$$
\sum_{a\in\mathcal{G}} D^{(\alpha)}_{ij}(a) D^{(\beta)}_{kl}(a^{-1}) = \frac{g}{d_\alpha}\delta_{\alpha\beta}\delta_{ij}\delta_{kj}.
$$

Often we are only intrested in studying the characters of some irreducible representation. We can form the traces of the represented elements by mutiplying both sides by $\delta_{ij}\delta_{kl}$, and taking the sum over k and l,

$$
\begin{aligned}
&\sum_{ik}\sum_{a\in\mathcal{G}} D^{(\alpha)}_{ii}(a) D^{(\beta)}_{kk}(a^{-1}) = \frac{g}{d_\alpha}\delta_{\alpha\beta}\underbrace{\sum_{ik}\delta_{ik}\delta_{ki}}_{d_\alpha} \\
\Rightarrow \quad &\sum_{a\in\mathcal{G}} \chi^{(\alpha)}(a)\chi^{(\beta)}(a^{-1}) = g\delta_{\alpha\beta}.
\end{aligned}
$$

From the preservation of the composition law of the representation $D(a^{-1}) = D^{(-1)}(a)$, and if the representation is unitary, which is allways possible to find, we have $D(a^{-1}) = D^{\dagger}(a)$. The trace is then $\chi(a^{-1}) = \chi(a)^*$, which simplifies our expression to

$$\sum_{a\in\mathcal{G}} \chi^{(\alpha)}(a)\chi^{(\beta)}(a)^* = g\delta_{\alpha\beta}.$$

For a reducible representation, with some character χ, we can decompose it as a sum over characters of irreducible representations

$$\chi(\mathcal{G}) = \sum_{\alpha} m_\alpha \chi^{\alpha}(\mathcal{G}).$$

where m_α is the number of identical representations. So we can find a more general relation

$$\sum_{a\in\mathcal{G}} \chi(a)\chi^{(\beta)}(a^{-1}) = \sum_{a\in\mathcal{G}}\sum_{\alpha} m_\alpha \chi^{(\alpha)}(a)\chi^{(\beta)}(a^{-1}) = \sum_{\alpha} m_\alpha g\delta_{\alpha\beta} = m_\beta g$$

so we find the multiplicity do be determined by

$$\begin{aligned} m_\alpha &= \frac{1}{g}\sum_{a\in\mathcal{G}} \chi(a)\chi^{(\alpha)}(a^{-1}) \\ &= \frac{1}{g}\sum_{a\in\mathcal{G}} \chi(a)\chi^{(\alpha)}(a)^* \\ &= \frac{1}{g}\sum_{i=1}^{n} r_i\chi(K_i)\chi^{(\alpha)}(K_i)^* \end{aligned}$$

where r_i are the number of elements in the class K_i and n is the number of classes.

Example 15. The characters of the classes of C_{3v}

We have earlier found the characters for the elements of C_{3v} so now we easily find the characters for their corresponding classes

$$\begin{aligned} \chi(e) = 3 &\implies \chi(K_1) = 3,\ r_1 = 1, \\ \chi(c_3) = 0 &\implies \chi(K_1) = 0,\ r_2 = 2, \\ \chi(\sigma_1) = 1 &\implies \chi(K_1) = 1,\ r_3 = 3, \end{aligned} \tag{2}$$

■

Another relation that is usable is

$$\begin{aligned} \sum_{a\in\mathcal{G}} |\chi(a)|^2 &= \sum_{a\in\mathcal{G}}\sum_{\alpha\beta} \left(m_\alpha\chi^{(\alpha)}(a)\right)\left(m_\beta\chi^{(\beta)}(a)\right) \\ &= \sum_{\alpha\beta}\sum_{a\in\mathcal{G}} \left(\chi^{(\alpha)}(a)\chi^{(\beta)}(a)^*\right) m_\alpha m_\beta = \sum_{\alpha\beta} g m_\alpha m_\beta \delta_{\alpha\beta} \\ &= g\sum_{\alpha} m_\alpha^2. \end{aligned}$$

Remark that the sum over all the multiplicities are allways greater or equal to one, i.e.

$$\sum_{\alpha} m_{\alpha}^2 \geq 1$$

with equal if and only if $m_\alpha = 1$ for one irreducible representation and zero for all others.

Theorem 2.

- A representation is irreducible if and only if

$$\sum_{a \in \mathcal{G}} |\chi(a)|^2 = \sum_{a=1}^{n} |\chi(K_a)|^2 r_a = g.$$

- The number of inequivalent irreducible representations is identicla to the number of classes.
- Burnside's thorem states that

$$\sum_{\alpha=1}^{n} (\dim \alpha)^2 = g.$$

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Example 16. "Triangular functions"-representation

Let $\mathcal{L} = \text{span}\{f_1, f_2, f_3\}$, so $\dim \mathcal{L} = 3$, and $\mathcal{L}$ is a Hilbertspace. We will now verify the characters of C_{3v}, earlier found, c.f. (2), but now using our newly found relations.

First we check if the representation is reducible

$$\sum_{a=1}^{3} r_a |\chi(K_a)|^2 = 1 \times 9 + 2 \times 0 + 3 \times 1^2 = 12 > 6 = \text{ord}\, C_{3v}$$

which it apperently is.

Remember from examples 13 and 14 that

$$\begin{array}{ll} \chi^{(1)}(K_1) = 1, & \chi^{(2)}(K_1) = 2 \\ \chi^{(2)}(K_2) = 1, & \chi^{(2)}(K_2) = -1 \\ \chi^{(3)}(K_3) = 1, & \chi^{(2)}(K_3) = 0 \end{array}$$

with multiplicities

$$\begin{aligned} m_1 &= \frac{1}{6}(3 \times 1 \times 1 + 0 + 1 \times 1 \times 3) = 1 \\ m_2 &= \frac{1}{6}(3 \times 2 \times 1 + 0 + 1 \times 0) = 1 \end{aligned}$$

are the characters of the irreducible representations. So if there are no more irreducible representations we can write this representation as

$$D(\mathcal{G}) = D^{(1)}(\mathcal{G}) \oplus D^{(2)}(\mathcal{G}).$$

We have 3 classes, therefor 3 inequivalent irreducible representations, so there is one more. We can see that $m_3 = 0$ since $d_1 + d_2 = \dim D$, so "there is no place left" fot the last one. But we can still find it. Through Burnsides theorem (theorem 2) we find

$$d_1^2 + d_2^2 + d_3^2 = 6 \Longrightarrow d_3^2 = 6 - 1 - 4 = 1$$

that the dimesion of the last representation is one. We can for the character table for C_{3v}

	K_1	K_2	K_3
1	1	1	1
2	2	-1	0
3	1	x	y

To find the two last characters, i.e. $\chi^{(3)}(K_2) = x$ and $\chi^{(3)}(K_3) = y$, we can use the orthogonality condition, i.e.

$$\sum_{a=1}^{n} r_a \chi^{(\alpha)}(K_a) \chi^{(\beta)}(K_a)^* = 0; \quad \alpha \neq \beta$$

so using this with representations 1 & 3 and 2 & 3 respectively we get

$$\begin{aligned} 1 \times 1 \times 1 + 2 \times 1 \times x + 3 \times 1 \times y &= 0 \\ 2 - 2x &= 0 \quad \Rightarrow \quad x = 1 \Rightarrow y = -1 \end{aligned}$$

and thats all the characters for all irreducible representations of C_{3v}.

■

We can write the orthogonality reltaion in matrix form. Let

$$\mathbb{X}_{\alpha a} = \chi^{(\alpha)}(K_a) \sqrt{\frac{r_a}{g}}$$

so that we get

$$\mathbb{X}^\dagger_{a\alpha} = \mathbb{X}^*_{\alpha a} = \sqrt{\frac{r_a}{g}} \chi^{(\alpha)}(K_a)^{(*)}$$

where the first index defines collumns, and the second rows. Then we can write the orthogonality relation as

$$\mathbb{X}\mathbb{X}^\dagger = \mathbb{I}$$

or equivalently

$$\sum_a \mathbb{X}_{\alpha a} \mathbb{X}^{(*)}_{\beta a} = \delta_{\alpha\beta}.$$

Example 17. Cyclic groups The cyclic group C_n was defined as the group generated by c_n, that have the property that $c_n^n = e$. C_n is abelian, therefor it has n-classes, and we should be able to find n number of irreducible representations, all of dimension one.

$$\begin{aligned}\left(\chi^{(\alpha)(c_n)}\right)^n &= \chi^{(\alpha)}(c_n^n) = \chi^{(\alpha)}(e)\\ &= 1\end{aligned}$$

The characters that solve the above equation is

$$\chi^{(\alpha)}(c_n) = e^{2\pi i \frac{k}{n}}; \quad k = 0, \dots, n-1.$$

and generates all elements of C_n. Let us introduce the identity irreducible representation, denoted A_1, and apply the ortogonality relation with respect to α. This gives

$$\sum_{k=0}^{n-1} e^{2\pi i \frac{k}{n}} 1^* = \frac{1 - e^{2\pi i k}}{1 - e^{2\pi i \frac{1}{n}}} = 0$$

since to the most left we have a geometric sum and the zero is demanded by the orthogonality relation. The character table would be

	K_1	$\dots$	K_n
A_1	1	$\dots$	1
$\vdots$	$\vdots$		
A_n	1		

where all rows and collums are all different permutations of $e^{2\pi i \frac{k}{n}}$. The notation we use here, A for a one dimensional irreducible representation and E, T, G and H for succeeding higher dimensions are called Mulleken notation, and is what we will start use from here on.

■

Projection operators

We can devide the space of operations into the spaces of each irreducible representation

$$\mathcal{L} = \bigoplus_{\alpha} \mathcal{L}^{(\alpha)}$$

and $\{| \alpha_i \rangle\}_{i=1,\dots,\dim \mathcal{L}^{(\alpha)}}$ is a basis of $\mathcal{L}^{(\alpha)}$. When a operator of some irreducible representation acts on one of the basis vectors it will be contained in the space of that representation, i.e. we have

$$D(a)| \alpha_i \rangle = \sum_{j=1}^{\dim \alpha} D_{ji}^{(\alpha)}(a)| \alpha_j \rangle$$

a linear combination of the basis of that subspace.

Definition 17 (Projection operator)**.** The unitary operator

$$P_i^{(\alpha)} = \frac{\dim \alpha}{g} \sum_i D_{ii}^{(\alpha)}(a)^* D(a)$$

is called the *projection operator*, and projects any vector in $\mathcal{L}$ onto $|\ \alpha_i\ \rangle$. This is can be seen by using the orthogonality relation

$$\begin{aligned}
P_i^{(\alpha)} |\ \beta_j\ \rangle &= \frac{\dim \alpha}{g} \sum_{a \in \mathcal{G}} D_{ii}^{(\alpha)}(a)^* \left(D(a) |\ \beta_j\ \rangle \right) \\
&= \frac{\dim \alpha}{g} \sum_{a \in \mathcal{G}} D_{ii}^{(\alpha)}(a)^* \sum_k D_{kj}^{(\beta)}(a) |\ \beta_k\ \rangle \\
&= \frac{\dim \alpha}{g} \sum_k \left(\delta_{\alpha\beta} \delta_{ij} \delta_{ki} \frac{g}{\dim \alpha} \right) |\ \beta_k\ \rangle \\
&= \delta_{\alpha\beta} \delta_{ij} |\ \beta_i\ \rangle \, .
\end{aligned}$$

There is also a projection operator that projects onto the complete subset $\mathcal{L}$,

$$P^{(\alpha)} = \sum_i P_i^{(\alpha)} = \frac{\dim \alpha}{g} \sum_{a \in \mathcal{G}} \chi^{(\alpha)}(a)^* D(a).$$

■

Definition 18 (Shift operator)**.** Another useful operator is the *shift operator* that is defined by

$$S_{ij}^{(\alpha)} = \frac{\dim \alpha}{g} \sum_{a \in \mathcal{G}} D_{ij}^{(\alpha)}(a)^* D(a)$$

that

$$S_{ij}^{(\alpha)} |\ \beta_k\ \rangle = \delta_{\alpha\beta} \delta_{ij} |\ \beta_i\ \rangle$$

■

Remark the resemblance with the ladder/step operators in quantum mechanics, as they also generates the other basis vectors in $\mathcal{L}^{(\alpha)}$.

The projection operator is idempotent, i.e.

$$\left(P_i^{(\alpha)} \right)^2 = P_i^{(\alpha)}.$$

Point groups

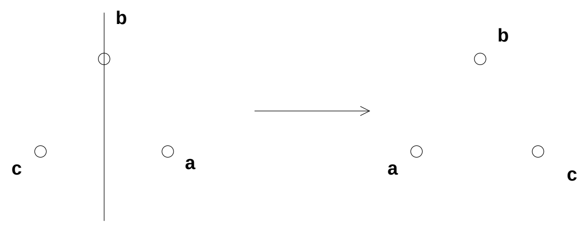
The groups we have studied so far are called *point groups*. A point group always consists of two types of elements:

- *Proper rotations*: c_n, which describes rotations around a n-fold axis.

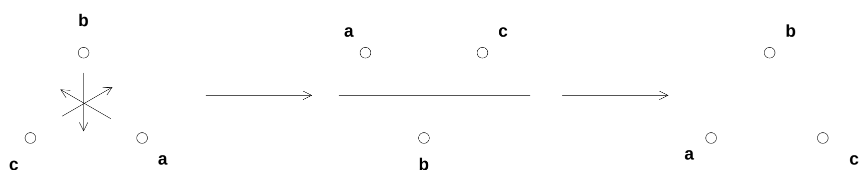
- *Improper rotations*: $c_n i$, where i is the inversion; $i\underline{x} = -\underline{x}$.

Example 18. Improper rotations in C_{3v}

When we acted with σ_b we mirrored the triangle as in the figure bellow.



But we can also represent the same action by a inversion and a 2-fold rotation, as illustrated bellow.



What we have concluded is $\sigma_b = c_2 i = i c_2$, and the same can be done for the other non-proper rotation elements in C_{3v}.

■

We donate the improper rotations either by $i_n = c_n i$ as rotation-inversions or by $s_n = c_n \sigma_n$ as mirrors.

Proper point groups

The proper point groups only contains elements of proper rotations, and there are five types of proper point groups.

- C_n: *The cyclic group*, is defined by $c_n^n = e$, and is Abelian and or order n.

- D_n: *The dihedral group*, defined by $c_n^n = e = c_2^2$, that is the symmetry has one n-fold axis and one 2-fold axis. This group has order $2n$ and the the number of classes are determined by
$$\frac{n+6}{2};\ \text{for even } n, \qquad \frac{n+3}{2};\ \text{for odd } n.$$

- T: *The tetrahedral group*, defined by $c_3^3 = c_2^2 = (c_3c_2)^3 = e$, that is the symmetry has four 3-fold axes and three 2-fold axes (three sided pyramid). The order of this group is 12 and has 4 classes.

- O: *The octahedral group*, defined by $c_4^4 = c_2^2 = (c_4c_2)^3 = e$, that is the symmetry has three 4-fold axes, four 3-fold axes and six 2-fold axes (the cube). The order is 24 and has 5 classes.

- Y: *The icosahedral group*, defined by $c_5^5 = c_2^2 = (c_5c_2)^3 = e$, that is the symmetry has six 5-fold axes, ten 3-fold axes and 15 2-fold axes. The order is 60 and the number of classes is 5.

Improper point groups

Improper point groups can be obtained in two ways, either as a outer direct product with $C_i = \{e, i\}$ or by decomposition of a proper point group into cosets with respect to a normal subgroup of index 2, i.e.
$$\mathcal{G}_p = \mathcal{H} \cup a\mathcal{H}$$
forms an improper point group $\mathcal{G}_p = \mathcal{H} \cup ia\mathcal{H}$.

In the first case the following new groups

$$C_n \longrightarrow \begin{cases} C_{nh} & ; n\text{even}, \\ S_{2n} & ; n \text{ odd}. \end{cases}$$
$$D_n \longrightarrow \begin{cases} D_{nh} & ; n\text{even}, \\ D_{nd} & ; n \text{ odd}. \end{cases}$$
$$T \longrightarrow T_h$$
$$O \longrightarrow O_h$$
$$Y \longrightarrow Y_h$$

where h and d stand for horizontal and diagonal, respectively, and is a fix index, different from n.

The other case we can find the following groups

$$\begin{aligned}
&C_{2n} \text{ w.r.t. } C_n \longrightarrow \begin{cases} C_{nh} & ; n \text{ even,} \\ S_{2n} & ; n \text{odd.} \end{cases} \\
&D_n \text{ w.r.t. } C_n \longrightarrow C_{nv} \\
&D_{2n} \text{ w.r.t. } D_n \longrightarrow \begin{cases} D_{nh} & ; n \text{ even,} \\ D_{nd} & ; n \text{odd.} \end{cases} \\
&O \text{ w.r.t. } T \longrightarrow T_d
\end{aligned}$$

The other does not have any normal subgroups.

Example 19. The finding of C_{3v} By looking at C_3 and D_3 we see that

$$\begin{aligned}
C_3 &= \{e, c_3, c_3^2\}, \\
D_3 &= \{e, c_3, c_3^2, c_2, c_2c_3, c_2c_3^2\} = \{e, c_3, c_3^2\} \cup c_2\{e, c_3, c_3^2\} = C_3 \cup c_2C_3.
\end{aligned}$$

So we find the C_{3v} group by

$$C_{3v} = C_3 \cup ic_2C_3 \cong C_3 \cup \sigma C_3.$$

■

Molecular vibrations

With a molecule consisting of N atoms, the position can be varried in $3N$ directions. So we should be able to find a representation of the point group in this displacement space, i.e. a $3N$ dimensional representation.

Example 20. The NH_3 molecule, with point group C_{3v} has four atoms, so we look for a 12-dimensional representation.

Displacement in Cartesian coordinates give us the representation as a direct group of atomic permutation on internal rotations. So our representation can be written

$$D(a) = D_{\text{at}}(a) \times D_{\text{int}}(a)$$

which has a trivial generalization to the N-atom case. For example

$$D(c_3) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

where the first matrix describes to which new places the atoms has been moved, and since c_3 is a rotation around the fourth atom, only the last column has its entry on the diagonal. And it has the character

$$\chi(c_3) = \text{Tr }(D_{at}(c_3)) \text{ Tr }(D_{\text{int}}(c_3)) = 0.$$

The character can be generalized to the expression

$$\chi(a) = \mathrm{Tr}\, D(a) = N_a \chi_{\mathrm{int}}(a)$$

where N_a is the number of atoms unmoved by the action of a. And

$$\chi_{\mathrm{int}}(a) = \begin{cases} 2\cos\theta + 1 & ;\text{proper } a = c_n, \\ 2\cos\theta - 1 & ;\text{improper } a = s_n \end{cases}$$

where θ measures the angle of rotation.

The other characters:

$$\chi(e) = 12$$
$$\chi(\sigma) = N_a \chi_{\mathrm{int}}(\sigma) = 2 \times 1 = 2.$$

		e	$2c_3$	3σ
$\Gamma^{(1)}$	A_1	1	1	1
$\Gamma^{(2)}$	A_2	1	1	-1
$\Gamma^{(3)}$	E	2	-1	0

And the corresponding multiplicities are found by the orthogonality relation

$$m_{A_1} = \frac{1}{g} \sum r_a \chi^{(A_1)}(K_a) \chi(K_a)^* = \frac{1}{6}(1 \times 12 + 2 \times 0 \times -1 + 6) = 3,$$
$$m_{A_2} = \frac{1}{6}(12 + 0 + (-6)) = 1,$$
$$m_E = \frac{1}{6}(24 + 0 + 0) = 4.$$

So our representation can be written

$$\bigoplus_{\alpha=1}^{3} m_\alpha \Gamma^{(\alpha)} = 3A_1 \oplus A_2 \oplus 4E.$$

Two types of atomic movements are uninteresting, that is those movement that simultaneously translates or rotates the whole molecule. Both these are three dimensional

$$\chi_{\mathrm{trans}}(a) = \begin{cases} 2\cos\theta + 1 & ; a = c_n \\ 2\cos\theta - 1 & ; a = s_n \end{cases} \quad \text{vector}$$
$$\chi_{\mathrm{rot}}(a) = \begin{cases} 2\cos\theta + 1 & ; a = c_n \\ -(2\cos\theta - 1) & ; a = s_n \end{cases} \quad \text{psedovector}$$

So for example

$$\chi_{\mathrm{trans}}(e) = 3 \quad \chi_{\mathrm{trans}}(c_3) = 0 \quad \chi_{\mathrm{trans}}(\sigma) = 1,$$
$$\chi_{\mathrm{rot}}(e) = 3 \quad \chi_{\mathrm{rot}}(c_3) = 0 \quad \chi_{\mathrm{rot}}(\sigma) = -1.$$

These are reducible

$$\begin{cases} [\text{Trans}] = A_1 \oplus E \\ [\text{Rot}] = A_2 \oplus E \end{cases}$$

The irreducible parts that are left forms the vibrations

$$[\text{Vib}] = 2A_1 \oplus 2E.$$

And in general we have that the character of the vibration is

$$\chi_{\text{vib}}(a) = \begin{cases} (N_a - 2)(2\cos\theta + 1) & ; a = c_n \\ N_a(2\cos\theta - 1) & ; a = s_n \end{cases}$$

■

Space groups

The space groups are groups of symmetry elements which brings a crystal onto itself. We represent the crystal as

$$\underline{R}(\underline{m}) + \underline{b}_i; \quad \underline{m} \in \mathbb{Z}^3$$

where $\underline{R}(\underline{m})$ is the crystal and $\{\underline{b}_i\}_{i=1,\ldots,d}$ is a basis.

Example 21. Consider one basis $\underline{b}_i = 0$, then the space group

$$\mathcal{G} = T^{(3)} \wedge \mathcal{G}_0$$

where $T^{(3)}$ consists of three dimensional translations and $\mathcal{G}_0$ is the point group that brings $\underline{R}(\underline{m}) \longrightarrow \underline{R}(\underline{m}')$. If $b \in \mathcal{G}_0$ then in a 3-dimensional representation we can represent the lattice in unit vectors $\{\underline{a}_i\}_{i=1,\ldots,3}$

$$\underline{R}(\underline{m}) = \sum_{i=1}^{3} m_i \underline{a}_i$$

■

We have that $\underline{m}' = D(b)\underline{m}$, and since all m_i are integers, we realize that

$$\chi(b) = \text{Tr}\,(D(b)) \in \mathbb{Z}.$$

And $\chi(b) = 2\cos\theta \pm 1 = k \in \mathbb{Z}$, so we deduce that $\theta \in \{0°, 60°, 90°, 120°, 180°, \ldots\}$, where these angles correspond to one-fold, six-fold, four-fold, three-fold and two-fold axises, respectively. Mark that there are no five- or seven-fold axis.

We have 7 possible point groups.

	Bravais lattices:	14
S_2:	triclinic	1
C_{2h}:	monoclinic	2
D_{2h}:	orthorhombic	4
D_{3d}:	rhombohedral	1
D_{4h}:	tetragonal	2
D_{6h}:	hexagonal	1
O_h:	cubic	3

We denote a element of a space group as $\{a|\underline{t}\} \in \mathcal{G}$, where a is a proper or improper rotation and $\underline{t}$ is the translation. This element acts on the radius vector $\underline{x}$ in the following way:

$$\{a|\underline{t}\}\underline{x} = D(a)\underline{x} + \underline{t}$$

where $D(a)$ is in the faithful representation.

There are some important algebraic rules

- $\{a|\underline{t}_1\}\{b|\underline{t}_2\} = \{ab|a\underline{t}_1 + \underline{t}_2\}$
- $\{a|\underline{t}\}^{-1} = \{a^{-1}| - a^{-1}\underline{t}\}$
- $\{a|0\} \in \mathcal{G}_0$, (a point group).
- $\{e|\underline{m}\} \in T^{(3)}$, (translational group).

A space group element $\{a|\underline{t}\}$ with $\underline{t} \notin T^{(3)}$ is called a **non-symmorphic** group element. However $\underline{t}^p \in T^{(3)};\ p \in \mathbb{Z}$.

We also see that $T^{(3)}$ always is a normal subgroup of the space group $\mathcal{G}$, since

$$\begin{aligned}
\{a|\underline{t}\}\{e|\underline{m}\}\{a|\underline{t}\}^{-1} &= \{a|a\underline{m} + \underline{t}\}\{a^{-1}| - a^{-1}\underline{t}\} \\
&= \{e| - aa^{-1}\underline{t} + a\underline{m} + \underline{t}\} \\
&= \{e|a\underline{m}\} \in T^{(3)}.
\end{aligned}$$

In general we can decompose $\mathcal{G}$ in terms of left or right cosets with respect to $T^{(3)}$

$$\mathcal{G} = \bigoplus_{i=1}^{h} \{a_i|\underline{t}_i\}T^{(3)} \tag{3}$$

where one element is the identity, say the first element, i.e. $\{a_1|\underline{t}_1\} = \{e|0\}$.

While $\{\{a|\underline{t}\}\}_{i=1,\ldots,h}$ generally does not form a group, but the set of point group elements $\{a_i\}_{i=1,\ldots,h}$ do form a point group, we call this the **isogonal** point group $\mathcal{G}_0$ with $\operatorname{ord}\mathcal{G}_0 = h$. However if $\forall \underline{t}_i = 0$, i.e. we only have symmorphic elements, then $\mathcal{G}_0 \subset \mathcal{G}$ and $\mathcal{G}$ can be written as

$$\mathcal{G} = T^{(3)} \wedge \mathcal{G}_0$$

and is a **symmorphic** space group.

We have several subgroups of the seven crystallographic groups. There are 73 symmorphic space groups. The non-symmorphic elements can be divided into two types

- **Glide planes:** $\{\sigma|\underline{t}\} \in \mathcal{G}$ and $\underline{t}^2 \in T^{(3)}$

- **Screw axis:** $\{c_n|\underline{t}\}$; $\{c_n|\underline{t}\}^n \in T^{(3)}$.

This provides 157 non-symmorphic space groups. So there are a total of 230 space groups with 32 different isogonal point groups.

Representations of space groups

Induced by $T^{(3)}$-abelian, normal subgroup gives 1-dim irreducible representations

$$T^{(3)} = T_1 \times T_2 \times T_3$$

along the unit vectors $\underline{a}_1, \underline{a}_2, \underline{a}_3$, respectively. We can impose a condition on T_i,

$$\{e|m_i\}^{N_i} = \{e|0\}$$

where $N_i >> 1$ is called the Born - von KÃ¡rmÃ¡n number, to make T_i cyclic. The character of the elements of this irreducible representation is then

$$\chi^{(n_i)}(\{e|m_i\})^{N_i} = 1 \quad ; n_i = 0, \ldots, N_{i-1}$$
$$\Rightarrow \quad \chi^{(n_i)}(\{e|m_i\}) = \exp\left(2\pi i \frac{m_i n_i}{N_i}\right)$$

or for $T^{(3)}$

$$\chi^{(\underline{n})}(\{e|\underline{m}\}) = \exp\left(2\pi i \sum_{j=1}^{3} \frac{m_j n_j}{N_j}\right)$$

Definition 19. The reciprocal lattice is a lattice $\underline{K}$ defined by

$$\underline{K} \cdot \underline{m} = 2\pi l; \quad l \in \mathbb{Z}$$

Expressed in the conjugate space basis

$$\underline{K} = \sum_{i=1}^{3} m_i^* \underline{a}_i^*; \quad m_i^* \in \mathbb{Z}$$

$$\text{where} \quad \underline{a}_i^* = 2\pi\epsilon_{ijk} \frac{\underline{a}_j \times \underline{a}_k}{\underline{a}_i \cdot \underline{a}_j \times \underline{a}_k}$$
$$\Rightarrow \quad \underline{a}_i \cdot \underline{a}_j^* = 2\pi\delta_{ij}$$

■

We can here introduce a wave vector

$$\underline{k} = \sum_{j=1}^{3} \frac{n_j}{N_j} \underline{a}_j^*; \quad n_j = 0, \ldots, N_{j-1}$$

inside the unit volume: $\underline{a}_i^* \cdot \underline{a}_j^* \times \underline{a}_k^* \epsilon_{ijk}$, called the Brillouin zone. Whence

$$\chi^{\underline{k}}(\{e|\underline{m}\}) = \exp\left(i\underline{k} \cdot \underline{R}(\underline{m})\right)$$

is the character of the irreducible representation $\underline{k}$ of $T^{(3)}$.

Let $\psi(\underline{k}, \underline{x})$ be the function spanning the 1-dim invariant subspace $\mathcal{L}^{\underline{k}}$, called the Bloch function

$$D^{(\underline{k})}(\{e|\underline{m}\})\psi(\underline{k}, \underline{m}) = \exp\left(i\underline{k} \cdot \underline{R}(\underline{m})\right) \psi(\underline{k}, \underline{x})$$

Using the coset decomposition of $\mathcal{G}$, (3) we can define the action of $\{a_i|\underline{t}_i\}$ on $\psi(\underline{k}, \underline{x})$. With the the faithful representation (a 3-dimensional real space) we get

$$D(\{a_i|\underline{t}_i\})\psi(\underline{k}, \underline{x}) = \psi(\underline{k}, \{e|\underline{t}_i\}^{-1}\underline{x}) = \psi(\underline{k}, a_i^{-1}(\underline{x} - \underline{t}_i)).$$

Since $\underline{k}$ and $\underline{x}$ are position vectors in two conjugate spaces (reciprocal and real, respectively) one can show (since $a_i^{-1} = a^T$, orthonormal) that

$$\psi(\underline{k}, a^{-1}(\underline{x} - \underline{t}_i)) = \psi(a\underline{k}, \underline{x} - \underline{t}_i).$$

We interpret this as rotation in real space corresponds to the inverse rotation in reciprocal space. This is a Bloch function too since

$$D(\{e|\underline{m}\})\psi(a\underline{k}, \underline{x} + \underline{t}) = \exp\left(ia\underline{k} \cdot \underline{R}(\underline{m})\right) \psi(a_i\underline{k}, \underline{x} - \underline{t}_i)$$

but it belongs to the irreducible representation $a_i\underline{k}$ and not $\underline{k}$.

Symmorphic

We have two cases

1. $a_i\underline{k} = \underline{k} \pmod{\underline{K}}$. This set of rotations $\{a_i\}$ form the *little cogroup* of $\underline{k}$, $\bar{\mathcal{G}}_{\underline{k}} \subset \mathcal{G}_0$.
2. $a_i\underline{k} = \underline{k}' \neq \underline{k} \pmod{\underline{K}}$. Then $\underline{k}'$ is said to belong to $\bigstar\underline{k}$, "star of $\underline{k}$". The order is

$$\operatorname{ord} \bigstar\underline{k} = \frac{\operatorname{ord} \mathcal{G}_0}{\operatorname{ord} \bar{\mathcal{G}}_{\underline{k}}}.$$

Irreducible Brillouin zone

For a general $\underline{k}$-point: $\operatorname{ord}\bar{\mathcal{G}}_{\underline{k}} = 1$ we have that

$$\dim \bigstar \underline{k} = \operatorname{ord}\mathcal{G}_0.$$

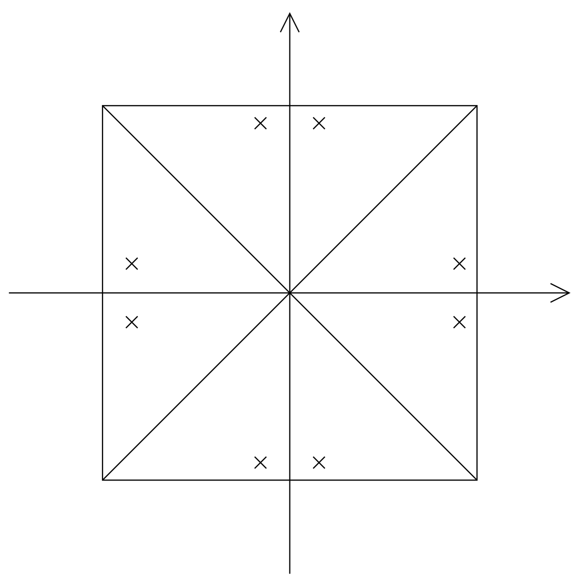
The $\frac{1}{\operatorname{ord}\mathcal{G}_0}$ part of the Brillouin zone contains all the information, since $a_i\underline{k} = \underline{k}'$ can be expanded to the whole zone.

For a limited set of $\underline{k}$'s, the $\bar{\mathcal{G}}_{\underline{k}}$ is non-trivial, we call these

$$-\text{symmetry}\begin{cases}\text{points}\\ \text{lines}\\ \text{planes}\end{cases}$$

on the wedge of IBZ.

Example 22. In the picture bellow the BZ is illustrated and we also see the $\underline{k}$ and $\underline{k}'$'s as crosses mirrored by the the mirror planes.



■

The dimensions of the irreducible representations are given by $\bar{\mathcal{G}}_{\underline{k}}$, which gives us a three dimensional representation.

In the non-symmorphic case a general $\underline{k}$-point is exactly the same. And symmetry points are determined by a case-to-case study of the irreducible representation of $\bar{\mathcal{G}}_{\underline{k}}$.

Example 23. Diamond structure Bravais lattice: face centered cubic (fcc). Basis:

$$\underline{b}_1 = [0,0,0]\,, \underline{b}_2 = \left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$$

in real space, expressed in units of $\underline{a}_i$. The corresponding reciprocal space is also cubic.

■

Spectroscopy

We are now going to study the matrix elements

$$\langle\, f \mid Q \mid i \,\rangle$$

that is a transition from an initial to an final state through the operator Q, e.g. a radiation field.

Assume we know that the system has the symmetry described by $\mathcal{G}$. And we know that all states can be labeled by irreducible representations of $\mathcal{G}$. In addition the operators can be decomposed into terms that transform according to the irreducible transformation.

In general we have $Q' = D(a)QD(a)^{-1}$ transformations. This can be decomposed into operators $\left\{Q_i^{(\alpha)}\right\}_{i=1,\ldots,d_\alpha}$ where each transforms according to its irreducible representation α, i.e.

$$\begin{aligned} Q'^{(\alpha)}_i &= D(a)Q^{(\alpha)}D(a)^{-1} \\ &= \sum_j D_{ji}^{(\alpha)} Q_j^{(\alpha)} \end{aligned}$$

Example 24. Radiation fields and its multipole expansion, the strongest term is usually the electric dipole. This translates as a vector, and can be either reducible or not. (e.g. T_2 of T_d)

■

In the most general case we have

$$\langle\, f\alpha \mid Q_j^{(\beta)} \mid i\gamma \,\rangle$$

where α, β and γ are irreducible representations of $\mathcal{G}$ and $j = 1, \ldots, d_\beta$. The first action is

$$\mid ji \,\rangle := Q_j^{(\beta)} \mid i\alpha \,\rangle$$

and

$$\begin{aligned} D(a)|\, ji\,\rangle &= D(a)Q_j^{(\beta)}D(a)^{-1}D(a)|\, i\alpha\,\rangle = \sum_{k,l} D_{kj}^{(\beta)}(a)Q_k^{(\beta)}D_{li}^{(\alpha)}(a)|\, l\alpha\,\rangle \\ &= \sum_{k,l} D_{kl,ji}^{(\beta\times\alpha)}(a)|\, kl\,\rangle\,. \end{aligned}$$

So we see that $|\, ji\,\rangle$ transforms according to the inner direct product representation $(\beta\times\gamma)$ which is in general reducible.

The character

$$\begin{aligned} \chi^{(\beta\times\gamma)}(a) &= \mathrm{Tr}\, D^{(\beta\times\gamma)}(a) = \sum_{k,l} D_{kl,kl}^{(\beta\times\gamma)}(a) \\ &= \sum_{k,l} D_{kk}^{(\beta)}(a)D_{ll}^{(\gamma)}(a) = \chi^{(\beta)}\chi^{(\gamma)} \end{aligned}$$

and hence

$$D^{(\beta\times\gamma)} = \bigoplus_{\alpha}^{\mathrm{IR}} m_\alpha D^{(\alpha)} = \bigoplus_{\alpha}^{\mathrm{IR}} (\beta\gamma|\alpha)D^{\alpha}$$

which is called the *Clebsch-Gordan decomposition*, and $(\beta\gamma|\alpha)$ are called the *reduction coefficient* which is

$$(\beta\gamma|\alpha) = \frac{1}{g}\sum_{a=1}^{n} r_a \chi^{(\beta)}(K_a)\chi^{(\gamma)}(K_a)\chi^{(\alpha)}(K_a)^*.$$

Example 25. $(\beta\gamma|\alpha) = (\gamma\beta|\alpha)$

C_{3v}	A_1	A_2	E
A_1	A_1	A_2	E
A_2	A_2	A_1	E
E	E	E	$A_1 \oplus A_2 \oplus E$

The first non-trivial element is $E \times A_2$, since it should be two dimensional, so it is either $A_1 \oplus A_2, E, 2A_1$ or $2A_2$, doing the explicit study it turns out to be E. Observe also that A_1 is always on the diagonal.

■

If we have the full representation then we need the Clebsch-Gordan coefficients

$$\left(\begin{array}{c|l} \beta\gamma & \alpha s \\ ij & k \end{array}\right)$$

where s determines which α since it is possible that there will be several, and $s = 1, \ldots, (\beta\gamma|\alpha)$, $i = 1, \ldots, d_\beta$, $k = 1, \ldots, d_\alpha$, $j = 1, \ldots, d_\gamma$. So now we have

$$\begin{aligned}
\langle\, f\alpha \mid Q_j^{(\beta)} \mid i\gamma \,\rangle &= \sum_{\alpha'} \sum_{s,k} \langle\, f\alpha \mid \left(\begin{array}{c|c} \beta\gamma & \alpha' s \\ ji & k \end{array} \right)^* \mid k\alpha'; s \,\rangle \\
&= \sum_{s} \langle\, f\alpha \mid k\alpha'; s \,\rangle \left(\begin{array}{c|c} \beta\gamma & \alpha' s \\ ji & k \end{array} \right)^* \delta_{\alpha\alpha'} \delta_{fk} \\
&= \sum_{s} \langle\, f\alpha \mid f\alpha : s \,\rangle \left(\begin{array}{c|c} \beta\gamma & \alpha s \\ ji & k \end{array} \right)^*
\end{aligned}$$

And matrix elements are zero whenever (α) is not in $(\beta \times \gamma)$. Also note that $\langle\, f\alpha \mid f\alpha; s \,\rangle$ is independent of i, j and f, since it is just a normalization factor.

Theorem 3. Wigner-Eckhart theorem

$$\langle\, f\alpha \mid Q_j^{(\beta)} \mid i\gamma \,\rangle = \sum \left(\begin{array}{c|c} \beta\gamma & \alpha s \\ ji & f \end{array} \right) \underbrace{\langle\, \alpha \mid |Q^{(\beta)}| \mid \beta \,\rangle}_{\text{reduced matrix elements}} .$$

■

In principle the symmetry group $\mathcal{G}$ can be a product of independent symmetries,

$$\mathcal{G} = \mathcal{G}_1 \times \mathcal{G}_2.$$

The irreducible representations of $\mathcal{G}$ are labeled by the the irreducible representations of $\mathcal{G}_1$ and $\mathcal{G}_2$ independently.

Often $\mid i\alpha \,\rangle$ is a many body system so one of the factor groups is the permutation group P_n.

Theorem 4. Cayleys theorem
Every group of $\operatorname{ord} \mathcal{G} = n$ is isomorphic to a subgroup of P_n.

■

Theorem 5. Any permutation can be decomposed in its independent cycles.

■

Example 26.

$$P_3 \cong C_{3v} \left\{ \begin{array}{lll} (123), (321) & K_2 & \text{cycles of 3} \\ (12)(3), (23)(1), (31)(2) & K_3 & \text{cycles of 2+1} \\ (1) & K_1 & \text{cycles of 1} \end{array} \right.$$

■

The classes can be labeled by $(\nu) = (\nu_1, \ldots, \nu_n)$ where ν_i is the number of i-cycles. Remark that

$$\sum_{i}^{\text{classes}} i\nu_i = n.$$

Example 27.

$$P_3 : \begin{cases} (3,0,0) & 3 \times 1 + 0 + 0 = 3 \\ (1,1,0) & 1 \times 1 + 1 \times 2 + 0 = 3 \\ (0,0,1) & 0 + 0 + 1 \times 3 = 3 \end{cases}$$

■

In the permutation group P_n there are the same number of irreducible representations as classes.

Definition 20.

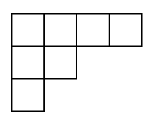
$$\lambda_k = \sum_{i=k}^{n} \nu_i; \quad [\lambda] = [\lambda_1, \ldots, \lambda_n]$$

■

Young diagram

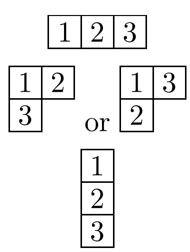
We can get the irreducible representations through Young-tableaux

$\lambda_1 = 4$
$\lambda_2 = 2$
$\lambda_3 = 1$



with $\lambda_i = 0$ for $i > 3$, and by then filling the boxes with integers $1, \ldots, n$ increasing both row and column.

Example 28. P_3 All possible diagrams



$[3]$1-dimensional (A_1)

$[2,1]$ 2-dimensional (E)

$[1^3] = [1,1,1]$ 1-dimensional (A_2)

■

There are always one irreducible representation $[n]$ and one $[1^n]$ called the *symmetric* and *anti-symmetric* representation, respectively.