Representation of point and space groups

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1 Overview of representations of finite groups

1.1 The characteristic table

The **character** of a group element in a representation is defined as its trace. Thus the character of e (i.e. the identity transform) is the dimension of the representation space.

Because $\operatorname{tr} gag^{-1} = \operatorname{tr} g^{-1}ga = \operatorname{tr} a$, we have

> **Character of conjugacy class**
>
> The characters of all elements in a conjugacy class are the same. (But having the same character doesn't mean two elements are in one conjugacy class.)

The **character table** is square, because

> **Number of irreducible representations**
>
> The number of conjugacy classes is the same as the number of irreducible representations.

Notation:

- The order of group G, i.e. the total number of elements it contains: n.
- p, q refer to labels of irreducible representations.
- g refers to a group element.
- $\chi^{(p)}(g)$ is the character of g in representation p.
- $[g]$ is the conjugacy class containing g.

> **The great orthogonality theorem**
>
> First,
>
> $$\frac{1}{n} \sum_{g \in G} \chi^{(p)}(g)^* \chi^{(q)}(g) = \delta_{pq}.$$
>
> Second, when g and g' are in the same conjugacy class,
>
> $$\frac{1}{n} \sum_{p} \chi^{(p)}(g)^* \chi^{(p)}(g') = \frac{1}{|[g]|},$$
>
> or otherwise the LHS vanishes.
> The second equation consequently means that the character table, if viewed as a matrix, is full rank.

The size of the conjugacy class of e is always 1, and therefore from the second equation above, we have

Burnside theorem

Suppose d_p is the dimension of the representation space of representation p.

$$\sum_p d_p^2 = n.$$

One usage of the character table:

Equivalent representations

Two representations are equivalent if and only if they have the same characters.

1.2 Representation of a group on a vector space

In physics we work with wave functions, operators, Hamiltonians, etc. We should note that when we say that a system has a symmetry G, it means for all operations U in G (or more precisely, in the representation of G on the Hilbert space),

$$\langle\psi|H|\varphi\rangle = \langle\psi|U^\dagger HU|\varphi\rangle \text{ for all } |\psi\rangle, |\varphi\rangle \Leftrightarrow H = U^\dagger HU, \tag{1}$$

and *not*

$$\langle\psi|H|\varphi\rangle = \langle\psi|U^\dagger UHU^\dagger U|\varphi\rangle,$$

because the latter is trivial true: it's like saying "when I rotate the system (i.e. H) and I rotate my experimental configurations (i.e. $|\psi\rangle$), the responses stay the same" – of course they *have to* say the same. A non-trivial claim would be something like "when I rotate my system, while *not* rotating my lab setup, magically all outputs are the same" – which is precisely (1).

1.3 Scalar, vector, tensor representations

Decomposition of tensor products

Because $\operatorname{tr} D_1(g) \otimes D_2(g) = \operatorname{tr} D_1(g) \operatorname{tr} D_2(g)$ for any group element g, the coefficients in

$$D_1(g) \otimes D_2(g) = \sum_p a_p D_p(g)$$

can be calculated by solving the equation system

$$\chi_{D_1}(g)\chi_{D_2}(g) = \sum_p a_p \chi_p(g)$$

for all conjugacy classes $[g]$. Note that the RHS is full-rank, and the equation has a unique solution.

2 Mulliken symbols

Representations of a group may be labeled as A_1, B_g, or things like that. This is known as the **Mulliken symbols**.

The A, B, E symbols mean the follows:

Table 1: Letter notation of dimension

dimension	**Mulliken symbol**
1	A and B
2	E
3	T
4	G
5	H

The distinction between A and B shows the sign of $\chi(c_n)$, where c_n represents rotation along the principal axis.

When an c_2 axis or a palne of reflection or a σ_v plane of reflection, we use subscripts $1, 2$ to indicate if a sign change follows after this operation. Similarly, g and u means $\chi(i) = \pm 1$, respectively. Finally, $\chi(\sigma_h)$ is represented by $'$ $(+1)$ or $''$ (-1).

3 How things changes under point group operations

Point group operations naturally have a representation in the 3D Euclidean space. This representation may be reducible: in this case, different irreducible representations act on different subspaces of $\mathbb{R}^3$.

We cannot know which subspace of $\mathbb{R}^3$ an irreducible representation acts on. Therefore in reference books, the standard character table is often augmented by what carries a representation.

Moreover, we note that some irreducible representations *cannot* be written as components of the natural representation on $\mathbb{R}^3$. The trivial identical representation of D_{3h}, for instance, doesn't correspond to how any subspace of $\mathbb{R}^3$ changes: we have σ_h and it's not possible to let z stay unchanged. These representations however can be carried by polynomials of x, y, z.

This website contains the extended character table of each point group.

4 Symmetry of dielectric tensor

In optics, $\boldsymbol{q}$ is usually small, and TODO: analyticity of ϵ

5 Optics in hexagonal crystals

Suppose we are dealing with a hexagonal system with D_{6h}. From the (extended; § 3) character table, we find that the A_{2u} irreducible representation acts on the z component, while the E_{1u} irreducible representation acts on the x, y components in $\mathbb{R}^3$. These can be known by consulting the character table here. Thus the representation of D_{6h} on $\mathbb{R}^3$ is

$$D = E_{1u} \oplus A_{2u}. \tag{2}$$

This is also given by the `dipole (p)` section of the webpage above. Note that strictly speaking, (2) does not track which components the representations act on: we need to keep that in mind ourselves.

Because we're working with optics, the wave length is assumed to be long enough, and in utilizing (1) (where the wave functions are replaced by electric field configurations, or "single-photon wave functions"), we can ignore the real space transform and focus on how components of $\boldsymbol{E}$ are mixed together. Thus (1) means that for all $g \in D_{6h}$,

$$\boldsymbol{\epsilon} = D^\dagger(g)\boldsymbol{\epsilon}D(g). \tag{3}$$

The RHS transforms as a rank-2 tensor. (TODO: covariant and contravariant indices?) The representation of D_{6h} it carries is $D \otimes D$. Note that the two D's cannot be exchanged, as the first acts on the first indices of ϵ_{ij}, while the second acts on the second indices. Keeping the meaning of being before and after $\otimes$, and that E_{1u} acts on the x, y component and A_{2u} acts on the z component (note that we have a natural z direction, which is parallel to the C_6 axis), we have

$$D \otimes D = (A_{2u} \otimes A_{2u}) \oplus (A_{2u} \otimes E_{1u}) \oplus (E_{1u} \otimes A_{2u}) \oplus (E_{1u} \otimes E_{1u}). \tag{4}$$

The next step is to see how the four tensor products act on the nine components of $\boldsymbol{\epsilon}$, following the procedure in § 1.3.

The ϵ_{zz} subspace We first notice that the absolute values of all characters of A_{2u} is 1, and hence the characters of $A_{2u} \otimes A_{2u}$ are all 1, meaning that

$$A_{2u} \otimes A_{2u} = A_{1g}, \tag{5}$$

i.e. the trivial representation. This immediately means that the ϵ_{zz} component is constant regardless of whatever operations applied to the system.

The $(\epsilon_{xz}, \epsilon_{yz})$ subspace By calculating the characters we also find

$$E_{1u} \otimes A_{2u} = E_{1g}. \tag{6}$$

This means the $\epsilon_{xz}, \epsilon_{yz}$ components transform as E_{1g}. Actually, once we realize that one irreducible representation acts on the x, y coordinates and another acts on the z coordinate, we should realize that $\epsilon_{xz}, \epsilon_{yz}$ transforms in the same way as xz, yz does: in the latter, the first variable (x or y) feels the action of E_{1u}, and the second variable (z) feels the action of A_{2u}. So indeed in the character table we find that E_{1g} acts on the space spanned by linearly recombining quadratic functions (xz, yz).

Now, from (1), we have

$$E_{1g}(g) \begin{pmatrix} \epsilon_{xz} \\ \epsilon_{yz} \end{pmatrix} = \begin{pmatrix} \epsilon_{xz} \\ \epsilon_{yz} \end{pmatrix}, \tag{7}$$

for all $g \in D_{6h}$. Because we know E_{1g} is D_{6h}'s action on the linear space spanned by (xz, yz), it immediately follows that

$$E_{1g}(c_6) = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, \tag{8}$$

and from that we find that the linear equation system in (7) only has a vanishing solution. This means in a hexagonal system, $\epsilon_{xz} = \epsilon_{yz} = 0$.

Following the same logic it can be shown that

$$\epsilon_{xz} = \epsilon_{yz} = \epsilon_{zx} = \epsilon_{zy} = 0. \tag{9}$$

What we have shown here is that the subspace of $\boldsymbol{\epsilon}$ that carries the $E_{1u} \otimes A_{2u}$ representation can't satisfy so many requirements from (1), and everything has to vanish.

The $\epsilon_{x/y,x/y}$ subspace