1.3: Irreducible Representations and Character Tables

Similarity transformations yield **irreducible representations**, Γ_i, which lead to the useful tool in group theory – the **character table**. The general strategy for determining Γ_i is as follows: **A**, **B** and **C** are matrix representations of symmetry operations of an arbitrary basis set (i.e., elements on which symmetry operations are performed). There is some similarity transform operator such that

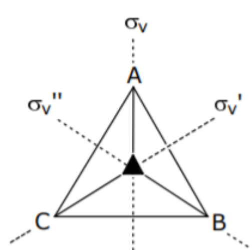
$$\begin{aligned} \boldsymbol{A}' &= v^{-1} \cdot \boldsymbol{A} \cdot v \\ \boldsymbol{B}' &= v^{-1} \cdot \boldsymbol{B} \cdot v \\ \boldsymbol{C}' &= v^{-1} \cdot \boldsymbol{C} \cdot v \end{aligned} \tag{1.3.1}$$

where *v* uniquely produces **block-diagonalized** matrices, which are matrices possessing square arrays along the diagonal and zeros outside the blocks

$$\mathbf{A}' = \begin{bmatrix} \mathrm{A}_1 & & \\ & \mathrm{A}_2 & \\ & & \mathrm{A}_3 \end{bmatrix} \quad \mathbf{B}' = \begin{bmatrix} \mathrm{B}_1 & & \\ & \mathrm{B}_2 & \\ & & \mathrm{B}_3 \end{bmatrix} \quad \mathbf{C}' = \begin{bmatrix} \mathrm{C}_1 & & \\ & \mathrm{C}_2 & \\ & & \mathrm{C}_3 \end{bmatrix} \tag{1.3.2}$$

Matrices **A**, **B**, and **C** are **reducible**. Sub-matrices A_i, B_i and C_i obey the same multiplication properties as **A**, **B** and **C**. If application of the similarity transform does not further block-diagonalize **A'**, **B'** and **C'**, then the blocks are **irreducible representations**. The **character** is the sum of the diagonal elements of Γ_i.

As an example, let's continue with our exemplary group: E, C_3, $C_3{}^2$, σ_v, σ_v', σ_v'' by defining an arbitrary basis … a triangle



The basis set is described by the triangles vertices, points A, B and C. The transformation properties of these points under the symmetry operations of the group are:

$$E \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} \quad \sigma_V \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} A \\ C \\ B \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} \tag{1.3.3}$$

$$C_3 \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} B \\ C \\ A \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} \quad \sigma_V' \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} B \\ A \\ C \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} \tag{1.3.4}$$

$$C_3^2 \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} C \\ A \\ B \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} \quad \sigma_V'' \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} C \\ B \\ A \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} \tag{1.3.5}$$

These matrices are not block-diagonalized, however a suitable similarity transformation will accomplish the task,

$$v = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} & 0 \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \quad ; \quad v^{-1} = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

Applying the similarity transformation with C_3 as the example,

$$v^{-1}\cdot \boldsymbol{C}_3 \cdot v = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} & 0 \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

$$\begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix} = \boldsymbol{C}_3^*$$

if $v^{-1} \cdot \mathbf{C_3^*} \cdot v$ is applied again, the matrix is not block diagonalized any further. The same diagonal sum is obtained *though off-diagonal elements may change). In this case, $\mathbf{C_3^*}$ is an irreducible representation, Γ_i.

The similarity transformation applied to other reducible representations yields:

$$v^{-1}\cdot \mathbf{E} \cdot v = \mathbf{E}^* = \left[\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}\right] \qquad v^{-1}\cdot \mathbf{C_3}^2 \cdot v = \mathbf{C_3}^2{*} = \left[\begin{array}{c|cc} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{array}\right]$$

$$v^{-1}\cdot \boldsymbol{\sigma}_{\mathrm{v}} \cdot v = \boldsymbol{\sigma}_{\mathrm{v}}{}^* = \left[\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ 0 & 0 & -1 \end{array}\right] \qquad v^{-1}\cdot \boldsymbol{\sigma}_{\mathrm{v}}{}'' \cdot v = \boldsymbol{\sigma}_{\mathrm{v}}{}'^* = \left[\begin{array}{c|cc} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{array}\right] \tag{1.3.6}$$

$$v^{-1}\cdot \sigma_v{}' \cdot v = \sigma_v{}^* = \left[\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{array}\right]$$

As above, the block-diagonalized matrices do not further reduce under reapplication of the similarity transform. All are Γ_{irr} **s**.

Thus a 3 × 3 reducible representation, Γ_{red}, has been decomposed under a similarity transformation into a 1 (1 × 1) and 1 (2 × 2) block-diagonalized irreducible representations, Γi. The traces (i.e. sum of diagonal matrix elements) of the Γ_i's under each operation yield the **characters** (indicated by χ) of the representation. Taking the traces of each of the blocks:

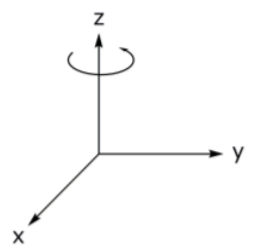
	E	C_3	$C_3{}^2$	σ_v	$\sigma_v{}'$	$\sigma_v{}''$
Γ_1	1	1	1	1	1	1
Γ_2	2	–1	–1	0	0	0

Note: characters of operators in the same class are identical

	E	$2C_3$	$3\sigma_v$
Γ_1	1	1	1
Γ_2	2	–1	0

This collection of characters for a given irreducible representation, under the operations of a group is called a **character table**. As this example shows, from a completely arbitrary basis and a similarity transform, a character table is born.

The triangular basis set does not uncover all Γ_{irr} of the group defined by {E, C_3, $C_3{}^2$, σ_v, σ_v', σ_v''}. A triangle represents Cartesian coordinate space (x,y,z) for which the Γ_is were determined. May choose other basis functions in an attempt to uncover other Γ_is. For instance, consider a rotation about the z-axis,



The transformation properties of this basis function, R_z, under the operations of the group (will choose only 1 operation from each class, since characters of operators in a class are identical):

$$\text{E: } R_z \rightarrow R_z \quad C_3 : R_2 \rightarrow R_2 \quad \sigma_v(xy) : R_2 \rightarrow \overline{R}_2$$

Note, these transformation properties give rise to a Γ_i that is not contained in a triangular basis. A new (1 x 1) basis is obtained, Γ_3, which describes the transform properties for R_z. A summary of the Γ_i for the group defined by E, C_3, $C_3{}^2$, σ_v, σ_v', σ_v" is:

	E	$2C_3$	$3\sigma_v$	
Γ_1	1	1	1	from triangular basis, i.e. (x, y, z)
Γ_2	2	−1	0	
Γ_3	1	1	−1	from R_z

Is this character table complete? Irreducible representations and their characters obey certain algebraic relationships. From these 5 rules, we can ascertain whether this is a complete character table for these 6 symmetry operations.

Five important rules govern irreducible representations and their characters:

Rule 1

The sum of the squares of the dimensions, ℓ, of irreducible representation Γ_i is equal to the order, h, of the group,

$$\sum_i \ell_i^2 = \ell_1^2 + \ell_2^2 + \ell_3^2 + \ldots = h$$

order of matrix representation of Γ_i (e.g. ℓ = 2 for a 2 × 2)

Since the character under the identity operation is equal to the dimension of Γ_i (since E is always the unit matrix), the rule can be reformulated as,

$$\sum_i \left[x_i(E) \right]^2 = h$$

character under E

Rule 2

The sum of squares of the characters of irreducible representation Γ_i equals h

$$\sum_R \left[x_i(R) \right]^2 = h$$

character of Γ_i under operation R

Rule 3

Vectors whose components are characters of two different irreducible representations are orthogonal

$$\sum_R \left[x_i(R)\right]\left[x_j(R)\right] = 0 \quad \text{for} \quad i \neq j$$

Rule 4

For a given representation, characters of all matrices belonging to operations in the same class are identical

Rule 5

The number of Γ_is of a group is equal to the number of classes in a group.

With these rules one can algebraically construct a character table. Returning to our example, let’s construct the character table in the absence of an arbitrary basis:

Rule 5: E (C_3, $C_3{}^2$) (σ_v, σ_v’, σ_v”) … 3 classes ∴ 3 Γ_is

Rule 1: $\ell_1^2+\ell_2^2+\ell_3^2=6 \quad \therefore \ell_1=\ell_2=1, \ell_2=2$

Rule 2: All character tables have a totally symmetric representation. Thus one of the irreducible representations, Γ_i, possesses the character set χ_1(E) = 1, χ_1(C_3, $C_3{}^2$) = 1, χ_1(σ_v, σ_v’, σ_v”) = 1. Applying Rule 2, we find for the other irreducible representation of dimension 1,

$$1 \cdot \chi_1(E) \cdot \chi_2(E) \;+\; 2 \cdot \chi_1(C_3) \cdot \chi_2(C_3) \;+\; 3 \cdot \chi_1(\sigma_v) \cdot \chi_2(\sigma_v) \;=\; 0$$

consequence of Rule 4

$$1 \cdot 1 \cdot x_2(E)+2 \cdot 1 \cdot x_2\left(C_3\right)+3 \cdot 1 \cdot x_2\left(\sigma_v\right)=0$$

Since χ_2(E) = 1,

$$1+2 \cdot x_2\left(C_3\right)+3 \cdot x_2\left(\sigma_v\right)=0 \quad \therefore \quad \chi_2\left(C_3\right)=1, \chi_2\left(\sigma_v\right)=-1$$

For the case of Γ_3 (ℓ_3 = 2) there is not a unique solution to Rule 2

$$2+2 \cdot \chi_3\left(C_3\right)+3 \cdot \chi_3\left(\sigma_v\right)=0$$

However, application of Rule 2 to Γ_3 gives us one equation for two unknowns. Have several options to obtain a second independent equation:

Rule 1: $1 \cdot 2^2+2\left[\chi_3\left(C_3\right)\right]^2+3\left[\chi_3\left(\sigma_v\right)\right]^2=6$

Rule 3: $1 \cdot 1 \cdot 2+2 \cdot 1 \cdot x_3\left(C_3\right)+3 \cdot 1 \cdot x_3\left(\sigma_v\right)=0$

or

$1 \cdot 1 \cdot 2+2 \cdot 1 \cdot x_3\left(C_3\right)+3 \cdot(-1) \cdot x_3\left(\sigma_v\right)=0$

Solving simultaneously yields $\chi_3\left(C_3\right)=-1, \chi_3\left(\sigma_x\right)=0$

Thus the same result shown on pg 4 is obtained:

$$\begin{array}{c|ccc} & \mathrm{E} & 2\mathrm{C}_3 & 3\sigma_{\mathrm{v}} \\ \hline \Gamma_1 & 1 & 1 & 1 \\ \Gamma_2 & 2 & -1 & 0 \\ \Gamma_3 & 1 & 1 & -1 \end{array} \tag{1.3.7}$$

Note, the derivation of the character table in this section is based solely on the properties of characters; the table was derived algebraically. The derivation on pg 4 was accomplished from first principles.

The complete character table is:

operations

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2$, z^2
A_2	1	1	−1	R_z	
E	2	−1	0	(x,y)(R_x,R_y)	($x^2 - y^2$, xy) (xz,yz)

Schoenflies symbol for point group

Mulliken symbols for the Γ_i

characters

basis functions

• Γ_is of:

$\ell = 1 \Longrightarrow A$ or B $\ell = 2 \Longrightarrow E$ $\ell = 3 \Longrightarrow T$	A is symmetric (+1) with respect to C_n B is antisymmetric (–1) with respect to C_n

- subscripts 1 and 2 designate Γ_is that are symmetric and antisymmetric, respectively to $\perp C_2$s; if $\perp C_2$s do not exist, then with respect to σ_v
- primes (’) and double primes (”) attached to Γ_is that are symmetric and antisymmetric, respectively, to σ_h
- for groups containing i, g subscript attached to Γis that are symmetric to i whereas u subscript designates Γis that are antisymmetic to i