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# Irreducible representations & character theory

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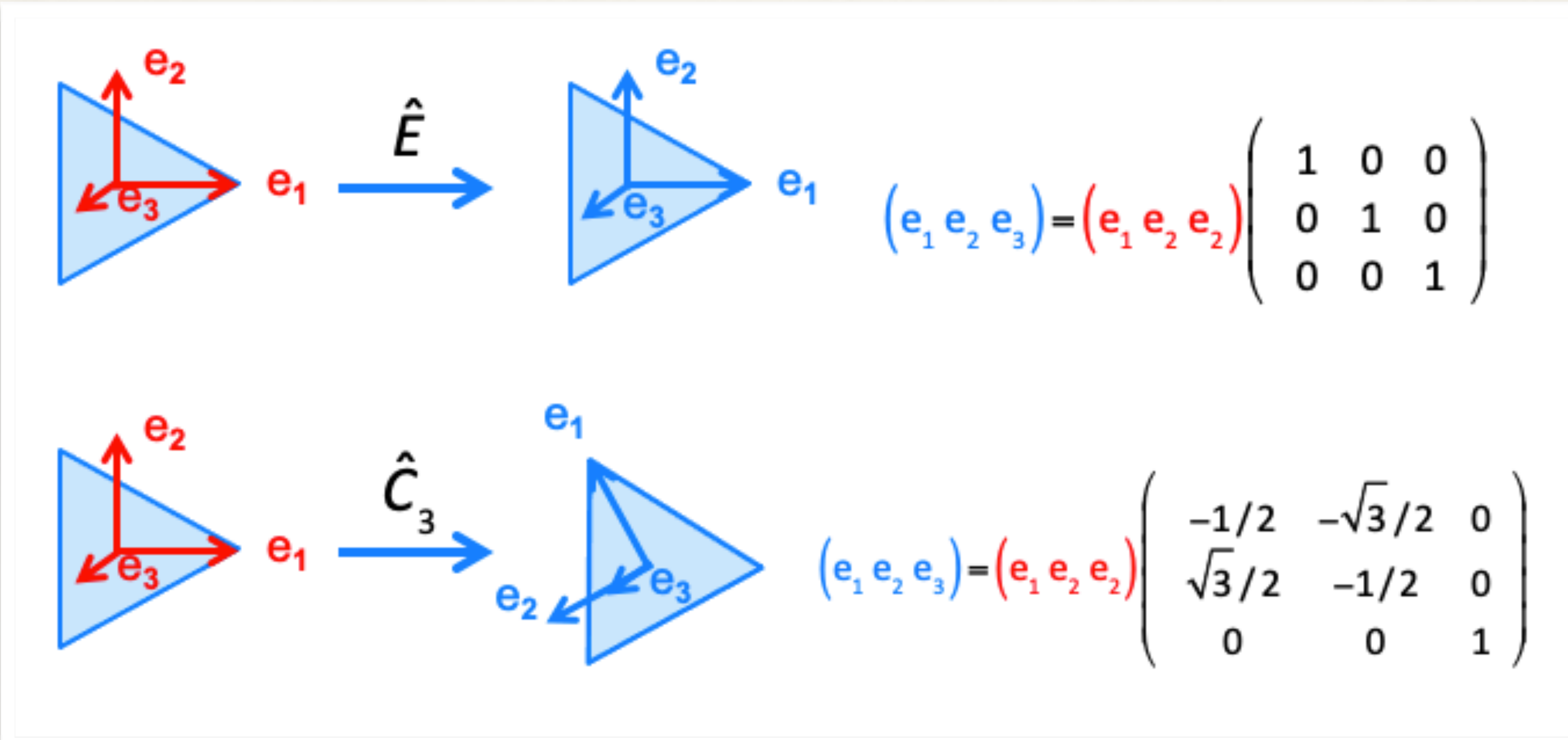
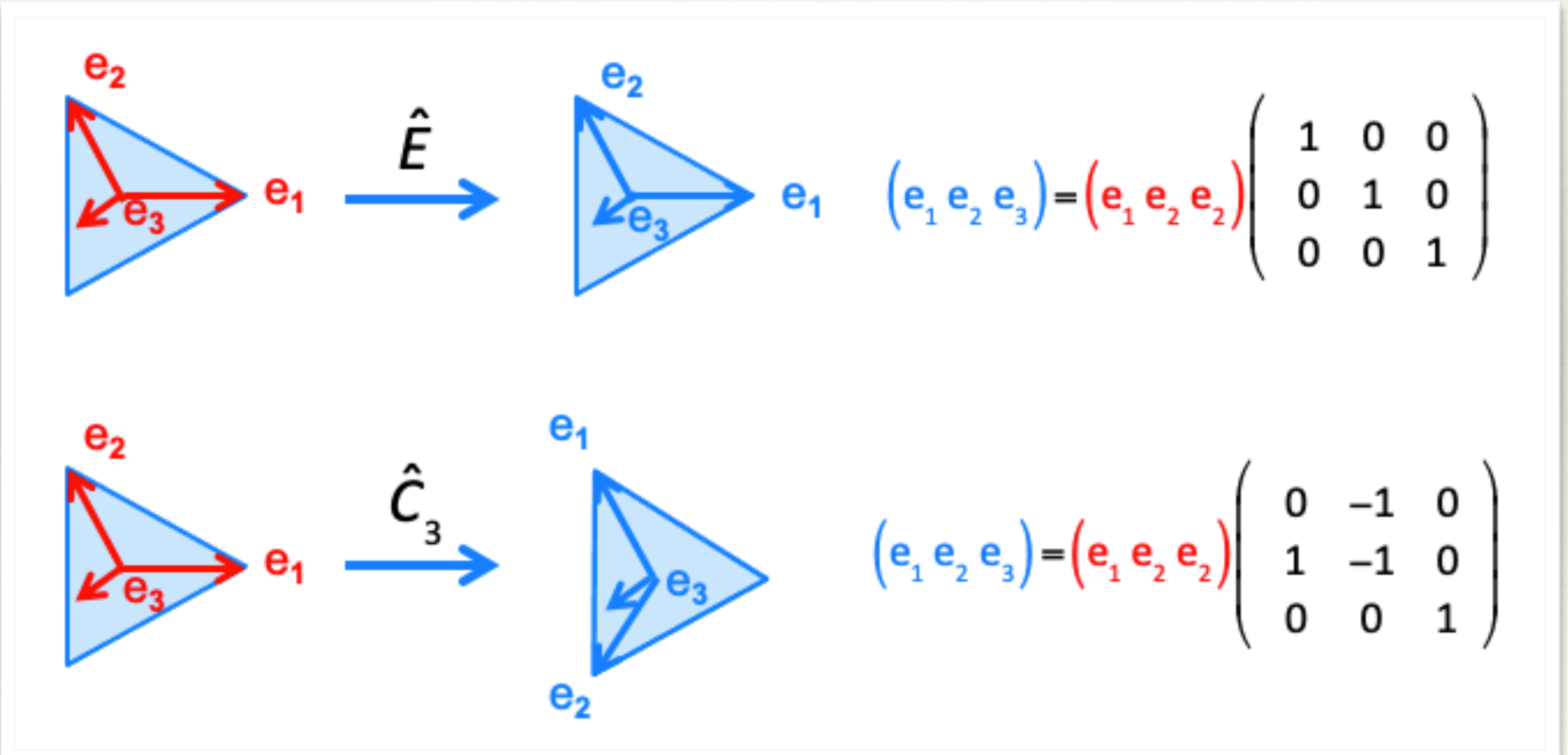
# $C_{3v}$ representations in $\mathbb{R}^3$

Let’s build a representation for $C_{3v}$ in $\mathbb{R}^3$ using the standard cartesian orthogonal basis



# $C_{3v}$ representations in $\mathbb{R}^3$

Now let's build the representation changing the basis in the sp{$e_1$,$e_2$} subspace to adapt it to the triangular symmetry



# Block-diagonal matrices

Using different basis sets we get two different representations for the $C_{3v}$ group. They are equivalent since they are related by a similarity transformation $\mathbf{A} = \mathbf{T}^{-1}\,\mathbf{B}\,\mathbf{T}$.

| $\hat{E}$ | $\hat{C}_3$ | $\hat{C}_3^2$ | $\hat{\sigma}_1$ | $\hat{\sigma}_2$ | $\hat{\sigma}_3$ |
|---|---|---|---|---|---|
| $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ |
| $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 1 & -1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ |

$$\left(\begin{array}{cc|c} R_{11} & R_{12} & 0 \\ R_{21} & R_{22} & 0 \\ \hline 0 & 0 & R_{33} \end{array}\right)$$

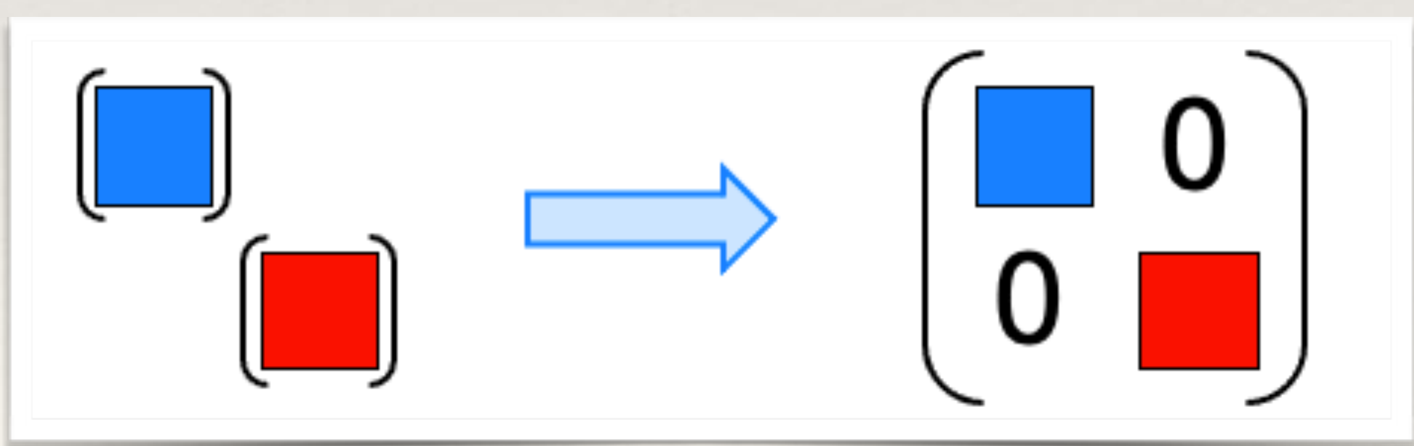
All matrices have the same **block-diagonal** shape

# Building large representations from smaller ones

For $C_{3v}$ we have found that there are only three fundamentally different representations

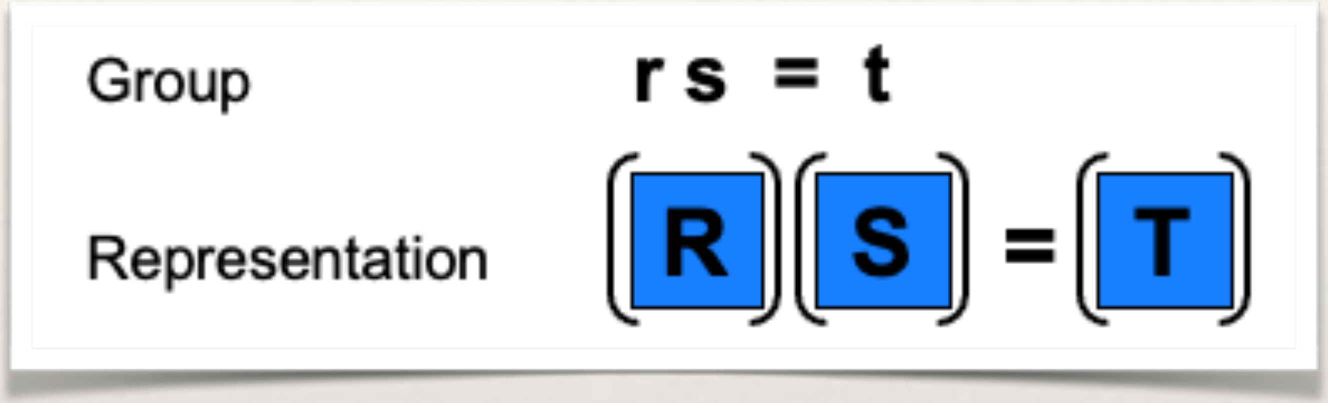
| | $\hat{E}$ | $\hat{C}_3$ | $\hat{C}_3^2$ | $\hat{\sigma}_1$ | $\hat{\sigma}_2$ | $\hat{\sigma}_3$ |
|---|---|---|---|---|---|---|
| $\Gamma_1$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $\Gamma_2$ | 1 | 1 | 1 | -1 | -1 | -1 |
| $\Gamma_3$ | $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix}$ |

Can we use them as basic elements to build larger representations?

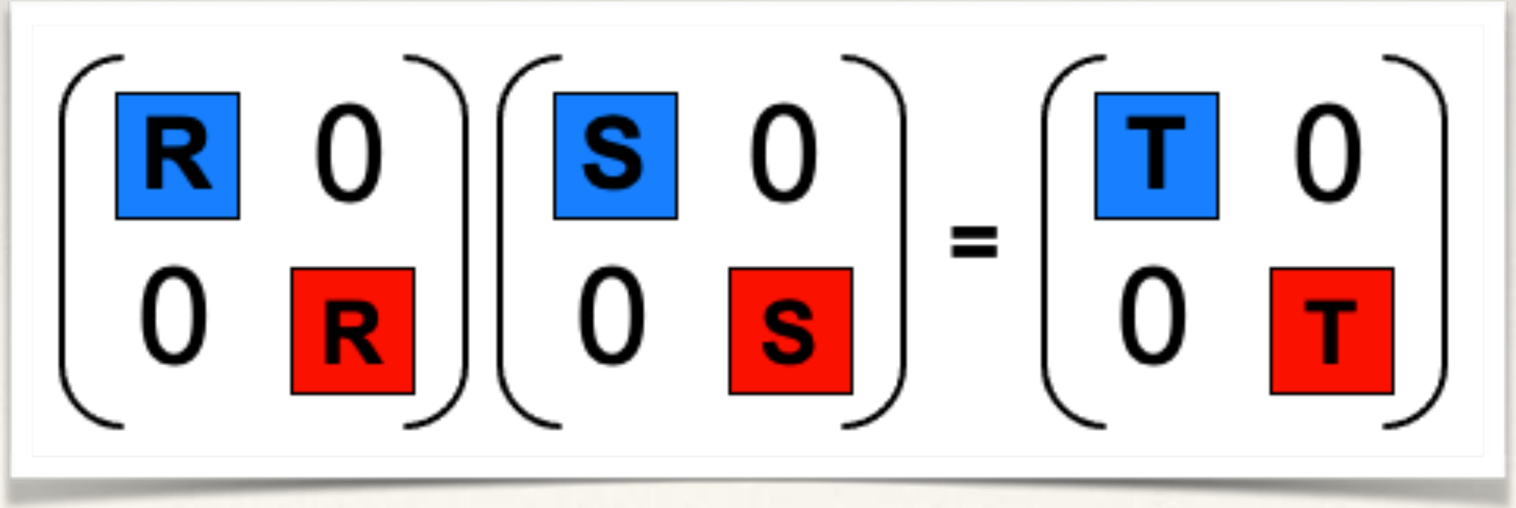


# Block-diagonal matrices preserve the group product

A group of matrices forms a representation if it has the same multiplication table as the original group elements:




If we build diagonal block matrices using smaller representations, the matrix product preserves the product of the individual blocks:

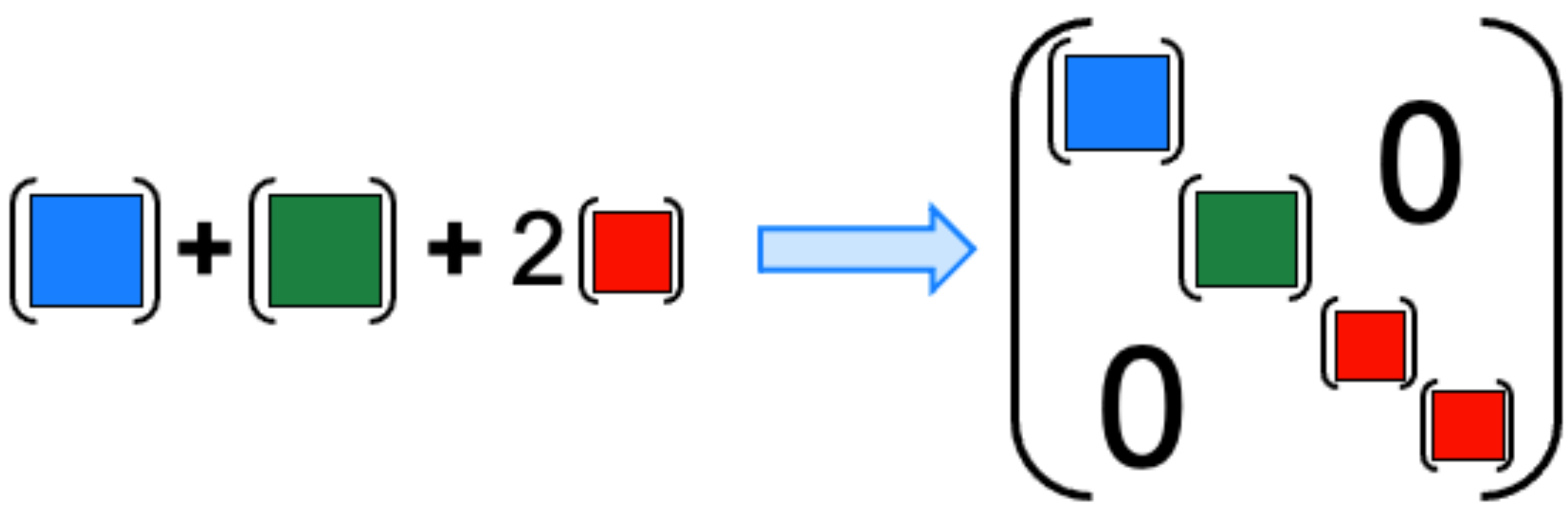



The diagonal block matrices form also a representation

# Direct sum of representations

A representation Γ obtained by building block-diagonal matrices of other representations $\Gamma_i$ is called the direct sum of all $\Gamma_i$

$$\Gamma = \Gamma_1 \oplus \Gamma_2 \oplus 2\Gamma_3$$



# Reduction of matrix representations

Our interest is really in simplifying representations, thus we are interested in reversing the above procedure:

$$D(R) = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \longrightarrow \bar{D}(R) = T^{-1} \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} T = \begin{pmatrix} \bar{R}_1 & 0 \\ 0 & \bar{R}_2 \end{pmatrix}$$

The process of finding representations of lower dimension whose direct sum is equivalent to a given representation is termed **reduction of a representation.**

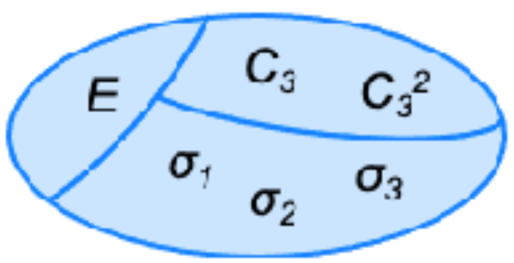
# Irreducible representations

Reduction can be repeated until the blocks can not be further reduced.

Representations whose matrices can not be simplified to block-diagonal form are called **irreducible representations** (IR) of the group

The search for simplest forms amounts to looking for non-equivalent IRs of dimension 1, 2, 3, …

… but we do not need to continue indefinitely,
since the number of IRs for any finite group is limited and determinable: it's equal to the number of conjugacy classes of the group!




| | $\hat{E}$ | $\hat{C}_3$ | $\hat{C}_3^2$ | $\hat{\sigma}_1$ | $\hat{\sigma}_2$ | $\hat{\sigma}_3$ |
|---|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | -1 | -1 | -1 |
| $E$ | $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$ | $\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$ | $\begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$ | $\begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix}$ | $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ |

# Orthogonality relations for representations

Let us consider the matrices of all IRs of a group

| | $\hat{E}$ | $\hat{C}_3$ | $\hat{C}_3^2$ | $\hat{\sigma}_1$ | $\hat{\sigma}_2$ | $\hat{\sigma}_3$ |
|---|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | -1 | -1 | -1 |
| $E$ | $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix}$ | $\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix}$ |

and build a set of vectors with the $R_{ij}$ elements

$$g_1 = (1,1,1,1,1,1) \qquad g_2 = (1,1,1,-1,-1,-1)$$
$$g_3 = (1,-1/2,-1/2,1,-1/2,-1/2) \qquad g_4 = (0,-\sqrt{3}/2,\sqrt{3}/2,0,-\sqrt{3}/2,\sqrt{3}/2)$$
$$g_5 = (0,\sqrt{3}/2,-\sqrt{3}/2,0,-\sqrt{3}/2,\sqrt{3}/2) \qquad g_6 = (1,-1/2,-1/2,-1,1/2,1/2)$$

The vectors are all orthogonal to each other! (this is true for any set of equivalent unitary IRs)

If $n_\alpha$ is the dimension of the $\Gamma_\alpha$ IR and $g$ the order of the group it seems also that:

$$\sum_\alpha n_\alpha^2 = g$$

# Character of a representation

The **trace of the matrix** which represents an element R of a group in a representation $\Gamma_\mu$ is called its character

$$\chi^{\mu}(R) = Tr\left\{\mathbf{D}^{\mu}(R)\right\}$$

The complete set of characters is called the **character of the representation**

| | $\hat{E}$ | $\hat{C}_3$ | $\hat{C}_3^2$ | $\hat{\sigma}_1$ | $\hat{\sigma}_2$ | $\hat{\sigma}_3$ |
|---|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | -1 | -1 | -1 |
| $E$ | 2 | -1 | -1 | 0 | 0 | 0 |

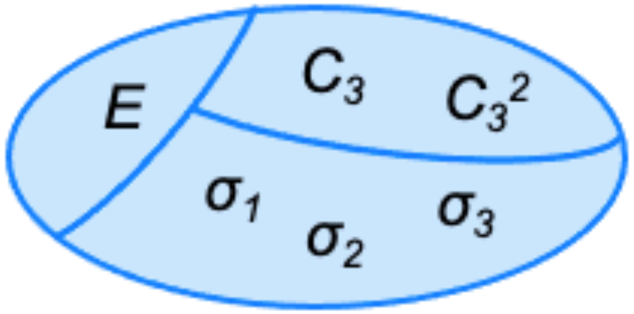
Since equivalent representations are related by a similarity transformation that preserves the trace of the matrices, the characters of two equivalent representations are identical

# Characters of conjugate elements

In any arbitrary representation, two elements conjugate to each other (two elements in the same class) have the same character

$$P = X^{-1} Q X \longrightarrow \chi^{\mu}(P) = \chi^{\mu}(Q)$$

| | $\hat{E}$ | $\hat{C}_3$ | $\hat{C}_3^2$ | $\hat{\sigma}_1$ | $\hat{\sigma}_2$ | $\hat{\sigma}_3$ |
|---|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | -1 | -1 | -1 |
| $E$ | 2 | -1 | -1 | 0 | 0 | 0 |




| | $\hat{E}$ | $2\hat{C}_3$ | $3\hat{\sigma}$ |
|---|---|---|---|
| $A_1$ | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | -1 |
| $E$ | 2 | -1 | 0 |

# Orthogonality relations for characters

Orthogonality relations for matrix elements of IRs lead to the existence of orthogonality relations for characters

| $C_{3v}$ | $\hat{E}$ | $2\hat{C}_3$ | $3\hat{\sigma}$ |
|---|---|---|---|
| $A_1$ | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | -1 |
| $E$ | 2 | -1 | 0 |

$$\sum_R \chi^{\mu}(R)\chi^{\nu}(R)^* = g\delta_{\mu\nu}$$

| | | |
|---|---|---|
| $\mu,\nu = A_1$ | $1\times1 + 2\times[1\times1] + 3\times[1\times1]$ | $= 6$ |
| $\mu,\nu = A_2$ | $1\times1 + 2\times[1\times1] + 3\times[(-1)\times(-1)]$ | $= 6$ |
| $\mu,\nu = E$ | $2\times2 + 2\times[(-1)\times(-1)] + 3\times[0\times0]$ | $= 6$ |
| $\mu=A_2,\nu = E$ | $1\times2 + 2\times[1\times(-1)] + 3\times[(-1)\times0]$ | $= 0$ |

# How many times does an IR appear in a RR?

Let us consider a reducible representation

$$\Gamma^{red} = a_1\Gamma^1 \oplus a_2\Gamma^2 \oplus \ldots \oplus a_\mu\Gamma^\mu \oplus \ldots \oplus a_k\Gamma^k \quad \longrightarrow \quad \chi^{red}(R) = \sum_{\nu=1}^{k} a_\nu \chi^\nu(R)$$

where $k$ is the number of classes ( = number of IRs) in the group

Multiplying on both sides by $\chi^\mu(R)^*$ and summing over all operations of the group:

$$\sum_R \chi^{red}(R)\chi^\mu(R)^* = \sum_R \sum_{\nu=1}^{k} a_\nu \chi^\nu(R)\chi^\mu(R)^* = \sum_{\nu=1}^{k} a_\nu g \delta_{\mu\nu} = g a_\mu$$

and therefore:

$$a_\mu = g^{-1} \sum_R \chi^{red}(R)\chi^\mu(R)^*$$

# Reducibility criterion

We can also use the orthogonality relations to check if a representation is irreducible or not.

If

$$\Gamma^{\alpha} = a_1\Gamma^1 \oplus a_2\Gamma^2 \oplus \ \ldots \ \oplus a_{\mu}\Gamma^{\mu} \oplus \ \ldots \ \oplus a_k\Gamma^k$$

is irreducible, then all $a_{\mu}$ coefficients are zero except one, that will be the unity. So, if $\Gamma^{\alpha}$ is irreducible, its characters must satisfy

$$a_{\alpha} = 1 = g^{-1}\sum_{R} \chi^{\alpha}(R)\chi^{\alpha}(R)^{*}$$

in other words, a representation is irreducible when:

$$\sum_{R} \chi^{\alpha}(R)\chi^{\alpha}(R)^{*} = g$$