

## Equivalent Representations

- Given a matrix representation  $D(g)$  we can find an equivalent representation by a similarity transformation

$$\underline{D}(g) = S^{-1} D(g) S \quad \text{or} \quad S^{-1} \underline{O}_g S = \underline{O}_g$$

Then  $\underline{D}(g)$  is also a matrix rep

$$\begin{aligned} \underline{D}(g_1) \underline{D}(g_2) &= S^{-1} D(g_1) S S^{-1} D(g_2) S \\ &= S^{-1} D(g_1) D(g_2) S \\ &= S^{-1} D(g_1 g_2) S = \underline{D}(g_1 g_2) \end{aligned}$$

- The trace of the matrix is known as the "character of the representation" with symbol  $\chi$

$$\chi(g) \equiv \text{Tr } D(g)$$

Note the trace or character is independent of any similarity transform

## Reducible Representations

- A representation of the group is completely reducible if through a similarity transformation it can be brought to block diagonal form for all  $D(g)$  of the representation

i.e. if

$$D(g) = \begin{pmatrix} / & & & \\ & / & & \\ & & / & \\ & & & / \end{pmatrix}$$

Then by change of basis

$$\underline{D}(g) = S D(g) S^{-1}$$

The new matrix is block diagonalized

$$\underline{D}(g) = \begin{pmatrix} / D^{(1)} / & 0 \\ \hline 0 & / D^{(2)} / \end{pmatrix} \equiv D^{(1)} \oplus D^{(2)}(g)$$

- If a representation can not be block diagonalized it is irreducible

- Finding the irreducible representations, and the decomposition, e.g.  $D(g) = D^{(1)}(g) \oplus D^{(2)}(g)$  is our chief task!

• A general reducible rep can be decomposed

$$D(g) = D^{(1)} \oplus D^{(1)} \oplus D^{(2)} \oplus D^{(2)} \oplus D^{(2)} \oplus \dots$$

$$= \sum 2 D^{(1)} \oplus 3 D^{(2)} \oplus \dots \equiv \sum_i a_i D^{(i)}$$

means

Formal Direct sum of irreducible reps.

$$D(g) = \begin{pmatrix} D_1 & & & & \\ & D_1 & & & \\ & & D_2 & & \\ & & & D_2 & \\ & & & & D_2 \end{pmatrix}$$

• The trace of this matrix is

$$\chi(g) = \sum_i a_i \chi^{(i)}(g)$$

the # of times  $D^{(i)}$  appears

trace of full matrix

trace of the irreducible reps matrices

- Normally if I have a vector in vector space  $V$

$$|V\rangle = v^a |e_a\rangle$$

Then the action of the group operations mixes the components of the vector

$$v^a \xrightarrow{g} D^a_b(g) v^a$$

- The reduction separates the vector space  $V$  into direct sum  $V = V_1 \oplus V_2$ . Each vector  $|\vec{V}\rangle$  can be written

$$|\vec{V}\rangle = |\vec{V}_1\rangle + |\vec{V}_2\rangle \quad |V_1\rangle \in V_1 \text{ and } |V_2\rangle \in V_2$$

- and the components of  $|\vec{V}_1\rangle$  do not mix with  $|\vec{V}_2\rangle$  under the with each other under the action of the group (though the components of  $|\vec{V}_1\rangle$  mix amongst itself).

The vector space  $V_1$  and  $V_2$  constitute invariant subspaces, i.e. the action of the group on a vector in  $V_1$  returns a vector in  $V_1$

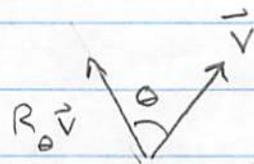
$$v_1^a \xrightarrow{g} D^{(1)a}_b v_1^b$$

$$v_2^{(a)} \xrightarrow{g} D^{(2)a}_b v_2^b$$

## Example of a reducible rep. Circular Polarization

- Consider the set of  $2 \times 2$  matrices representing the rotations around the  $Z$ -axis:

$$R_\theta \rightarrow \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = D(R_\theta)$$



This is a group (an abelian group)

$$R_\theta R_{\theta'} = R_{\theta + \theta'}$$

It is a continuous group (the number of elements is not fixed). Consider a change of basis of  $D(R_\theta)$

$$|\vec{e}_\pm\rangle \equiv \frac{\vec{e}_x \pm i\vec{e}_y}{\sqrt{2}}$$

$$\vec{v} = v_+^* \vec{e}_+ + v_-^* \vec{e}_-$$

$$|\vec{v}_\pm\rangle \equiv \frac{v_x \pm i v_y}{\sqrt{2}} = \frac{|\vec{v}|}{\sqrt{2}} (\cos\theta_v \pm i \sin\theta_v) = \frac{|\vec{v}|}{\sqrt{2}} e^{i\theta_v}$$

- So under rotation  $\theta_v \rightarrow \theta_v + \theta$  and thus

$$|\vec{v}_+\rangle \xrightarrow{R_\theta} \frac{|\vec{v}|}{\sqrt{2}} e^{i(\theta_v + \theta)} = e^{i\theta} |\vec{v}_+\rangle$$

$$|\vec{v}_-\rangle \xrightarrow{R_\theta} \frac{|\vec{v}|}{\sqrt{2}} e^{i(\theta_v + \theta)} = e^{-i\theta} |\vec{v}_-\rangle$$

Thus in our new basis we have the transformation

$$\begin{pmatrix} \underline{V}_+^* \\ \underline{V}_-^* \end{pmatrix} = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} \begin{pmatrix} V_+ \\ V_- \end{pmatrix}$$

$V_+$ ,  $V_-$  are known as the spherical components of a vector  $\vec{V}$ . They have the advantage over  $V^x, V^y$ . They transform as an irreducible representation under rotations.

- Under rotation one linearly polarization becomes another
- However one circularly polarized state just picks up a phase under rotations

## Some Theorems Without Proof

- ① The number of irreducible representations and their dimensions is very limited:

Let  $D^{(\mu)}(g)$  label the irreps with

$$\mu = 1, 2, \dots, N_{\text{reps}}$$

of dimension  $n_{\mu}$  ( $D^{(\mu)}$  is a  $n_{\mu} \times n_{\mu}$  matrix)

Then

$$\sum_{\mu=1}^{N_{\text{reps}}} n_{\mu}^2 = n_G$$

order of group = 6 for  $D_3$ , 3 for  $Z_3$

$$n_{\mu=1} = 1 \quad n_{\mu=1} = 1$$

We will later prove that identity, alternating, and matrix reps are the only irreps of  $D_3$ . Thus

$$n_{\mu=2} \uparrow$$

$$1^2 + 1^2 + 2^2 = 6$$

## ② Schur's Lemma I

Let  $D^{(\mu)}(g)$  be an irrep of dimension  $n_{\mu} \times n_{\mu}$ .  
Let  $A$  be a square matrix which commutes  
with  $D^{(\mu)}(g)$  for all  $g \in G$

$$[A, D^{(\mu)}(g)] = 0$$

Then either  $A = 0$  or  $A = \lambda \mathbb{1}$

Proof See Hammermesh (3.14)

### ③ Schur's Lemma 2

If  $D^{(1)}$  and  $D^{(2)}$  are two inequivalent reps of dimensions  $n_{(1)}$  and  $n_{(2)}$  respectively (can be different or same)

Then if a matrix  $A$  "intertwines"  $D^{(1)}$  and  $D^{(2)}$  meaning

$$D^{(1)}(g) A = A D^{(2)}(g) \quad \left( D^{(1)} \right) (A) = (A) \left( D^{(2)} \right)$$

Then  $A$  is zero.

④ Unitarity (for a finite, or compact group)  
Any matrix representation is equivalent to a unitary representation

A matrix is unitary if  $D^\dagger = D^{-1}$   $D^\dagger D = \mathbb{1}$   
Then a rep is unitary when

$$D_{ab}(g^{-1}) = (D^{-1}(g))_{ab} = (D^\dagger)_{ab} = (D^*)_{ba}$$

## The Great Orthogonality Theorem Without Proof

- Let the group have irreps  $D^{(\mu)}(g)$  with  $(\mu) = 1 \dots N_{\text{reps}}$  of dimension  $n_{\mu} \times n_{\mu}$
- Then the group averaged matrix elements are maximally orthogonal

$$\frac{1}{n_G} \sum_g D_{ab}^{(\mu)}(g) D_{cd}^{(\nu)}(g^{-1}) = \frac{1}{n_{\mu}} \delta_{\mu\nu} \delta_{ac} \delta_{bd}$$

Or since  $D$  is equivalent to a unitary rep

$$\frac{1}{n_G} \sum_g D_{ab}^{(\mu)}(g) (D_{cd}^{(\nu)}(g))^* = \frac{1}{n_{\mu}} \delta_{\mu\nu} \delta_{ac} \delta_{bd}$$

- We can phrase this like this. Consider "vectors" in the vector space of group operators. The notation is

$$\hat{V} = \sum_{i=1}^{n_G} v_i \hat{g}_i = \sum_i v_i \hat{g}_i = \sum_g v(g) \hat{g}$$

- We can add and subtract operators and take a "group" inner product

$$\langle \hat{V}, \hat{W} \rangle = \sum_{i=1}^{n_G} v_i^* w_i = \sum_g v^*(g) w(g)$$

Then define the "vectors" in this space of operators

$$\hat{e}_{ab}^{(\mu)} \equiv \left( \frac{n_\mu}{n_G} \right) \sum_g D_{ab}^{*(\mu)}(g) \hat{g}$$

$n_\mu/n_G$  inserted for later convenience

These vectors are orthogonal

$$\langle \hat{e}_{ab}^{(\mu)}, \hat{e}_{cd}^{(\nu)} \rangle = \frac{n_\mu}{n_G} \delta_{\mu\nu} \delta_{ac} \delta_{bd}$$

• Thus we have

$N_{\text{reps}}$

$$\sum_{\mu=1} n_\mu^2$$

orthogonal vectors in a "vector space" of dimension  $n_G$  we must have

$N_{\text{reps}}$

$$\sum_{\mu=1} n_\mu^2 \leq n_G$$

• In fact  $\sum n_\mu^2 = n_G$  and thus the vectors

$$\hat{e}_{ab}^{(\mu)}$$

Form a complete orthogonal basis for the group algebra (i.e. the group vector space)!

## Functions of Definite Symmetry

- Start with a function  $f$ . By acting on  $f$  with the group operator we get new functions

$$f, \quad f_1, \quad f_2, \quad f_3, \quad f_4, \quad f_5, \quad f_6$$
$$f, \quad O_{r_1}f, \quad O_{r_2}f, \quad O_{s_0}f, \quad O_{s_1}f, \quad O_{s_2}f$$

Then any function in the span of these functions is represented by the "vector",  $\hat{c} = c_i \hat{g}_i$

$$O_{\hat{c}} = \sum_i c_i \hat{O}_i = \sum_g C(g) \hat{O}_g$$

↑  
numbers

$$O_{\hat{c}} f = \sum_i c_i \hat{O}_i f$$

$$= \sum_i c_i f_i \quad \leftarrow \text{a function in the span}$$

- Instead of using the basis

$$f_i \equiv \hat{O}_i f$$

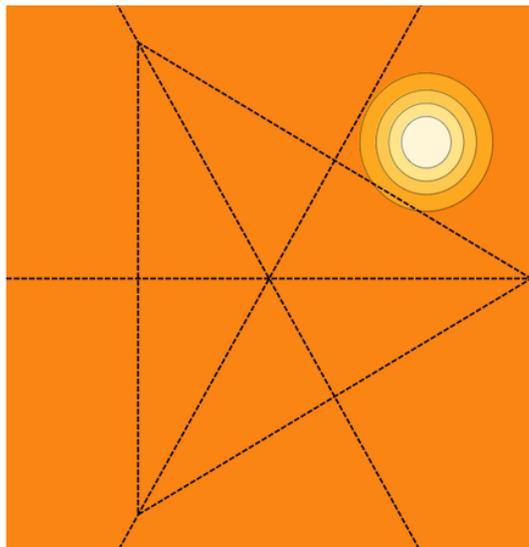
We will use

$$f_{ab}^{(\mu)} = \hat{e}_{ab}^{(\mu)} f = \frac{n_{\mu}}{n_G} \sum_i (D_{ab}^{(\mu)}(g_i))^* \hat{O}_{g_i} f$$

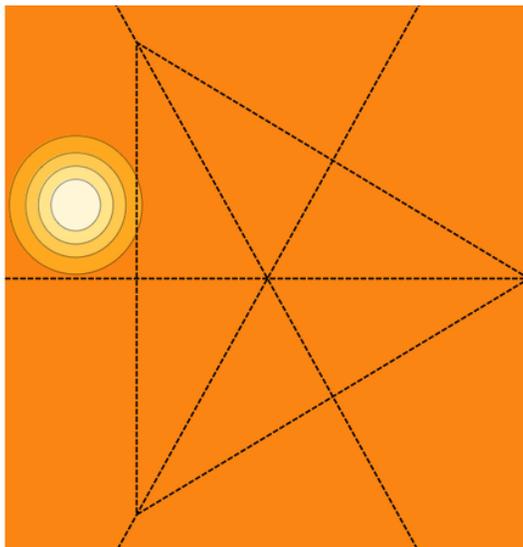
They have the same dimensionality

The vector space = linear span of six functions

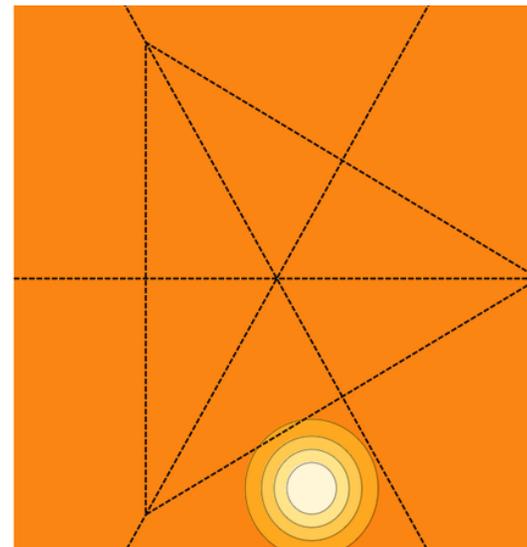
$f$



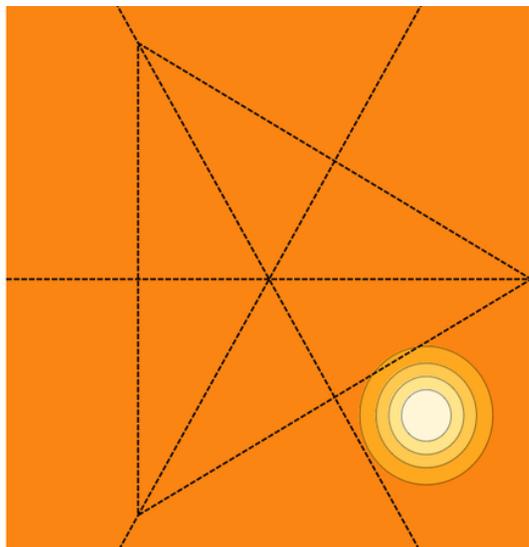
$O_{r_1} f$



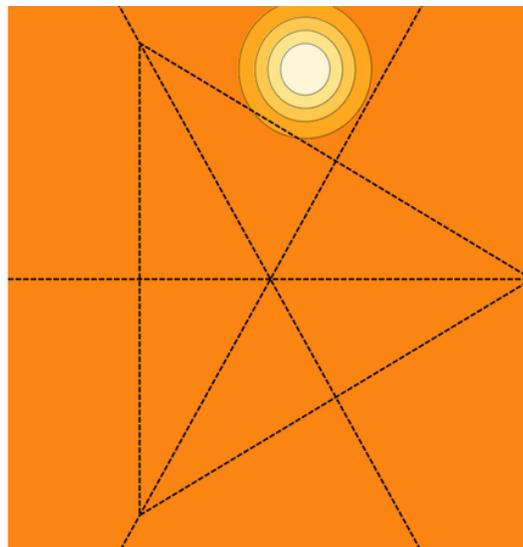
$O_{r_2} f$



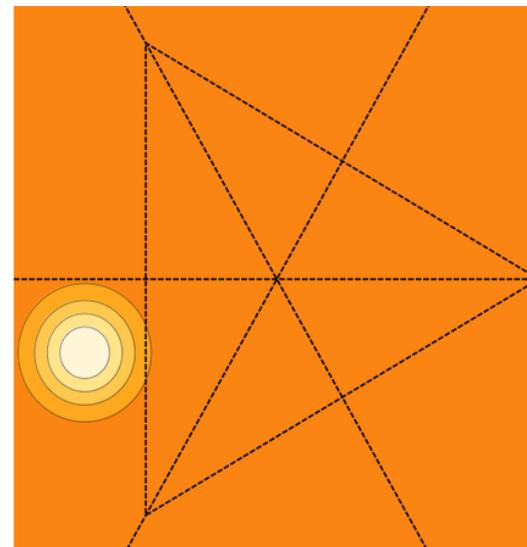
$O_{s_0} f$



$O_{s_1} f$



$O_{s_2} f$



• Take the identity rep  $n_{\mu} = 1$   $D_{\parallel}^{(\mu)}(g) = 1$

$$f_{\parallel}^{(1)} = \frac{1}{n_G} \sum_g O_g f$$

$$f_{\parallel}^{(1)} = \frac{1}{6} \sum_i f_i \quad \leftarrow \text{We looked this earlier } f_{\parallel}^{(1)} = f_s$$

This is invariant under the group ops

$$O_g f_{\parallel}^{(1)} = f_{\parallel}^{(1)}$$

• Similarly look at the alternating reps

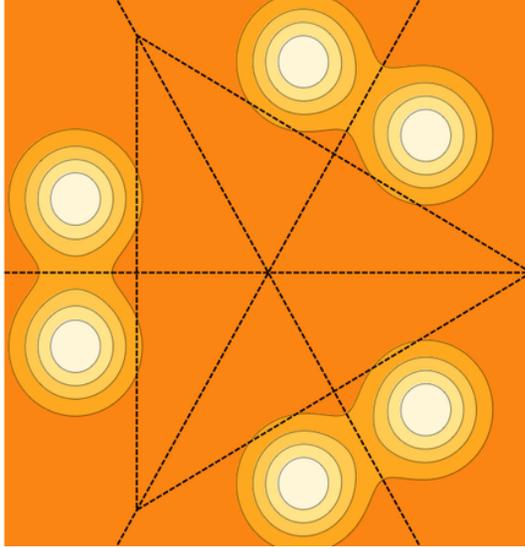
$$f_A = f_{\parallel}^{(2)} = \frac{1}{6} (f + O_{r_1} f + O_{r_2} f - O_{s_0} f - O_{s_1} f - O_{s_2} f)$$

Then <sup>this</sup> is, up to a sign, invariant:

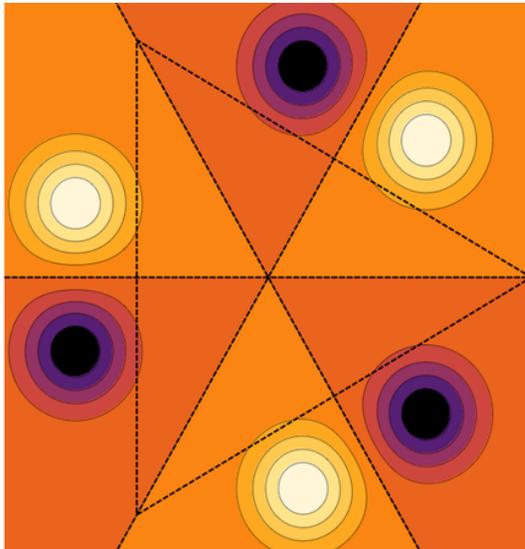
$$O_g f_{\parallel}^{(2)} = \pm f_{\parallel}^{(2)}$$

Where + is for  $O_{r_0}, O_{r_1}, O_{r_2}$  and - is for  $O_{s_0}, O_{s_1}, O_{s_2}$

These are shown on the slides



$$f_S(x) \equiv f_{11}^{(1)}(x)$$



$$f_A(x) \equiv f_{11}^{(2)}$$

- Now look at  $f_{11}^{(3)}$  and  $f_{21}^{(3)}$

$$f_{11}^{(3)} = \frac{1}{n_G} \sum_g (D_{11}^{(3)}(g))^* O_g f$$

$$f_{11}^{(3)} = \frac{2}{6} \left( f - \frac{1}{2} O_{r_1} f - \frac{1}{2} O_{r_2} f + O_{s_0} f - \frac{1}{2} O_{s_1} f - \frac{1}{2} O_{s_2} f \right)$$

Where we read of the blue matrix elements from the table on the next page. Similarly

$$f_{21}^{(3)} = \frac{2}{6} \left( \frac{\sqrt{3}}{2} O_{r_1} f - \frac{\sqrt{3}}{2} O_{r_2} f + \frac{\sqrt{3}}{2} O_{s_1} f - \frac{\sqrt{3}}{2} O_{s_2} f \right)$$

- We also construct

$$f_{12}^{(\mu)} \text{ and } f_{22}^{(\mu)}$$

- The functions

$$f_{a1}^{(\mu)} = \left\{ f_{11}^{(\mu)}, f_{21}^{(\mu)} \right\}$$

Are partners in an irreducible rep  $\mu=3$ . They span an invariant subspace in the span of the six original functions  $\{ f, O_{r_1} f, O_{r_2} f, O_{s_0} f, O_{s_1} f, O_{s_2} f \}$

- Similarly  $f_{a2}^{(\mu)} = \{ f_{12}^{(\mu)}, f_{22}^{(\mu)} \}$  are partners in an irrep.

### $D_3$ Matrix Representation Summary

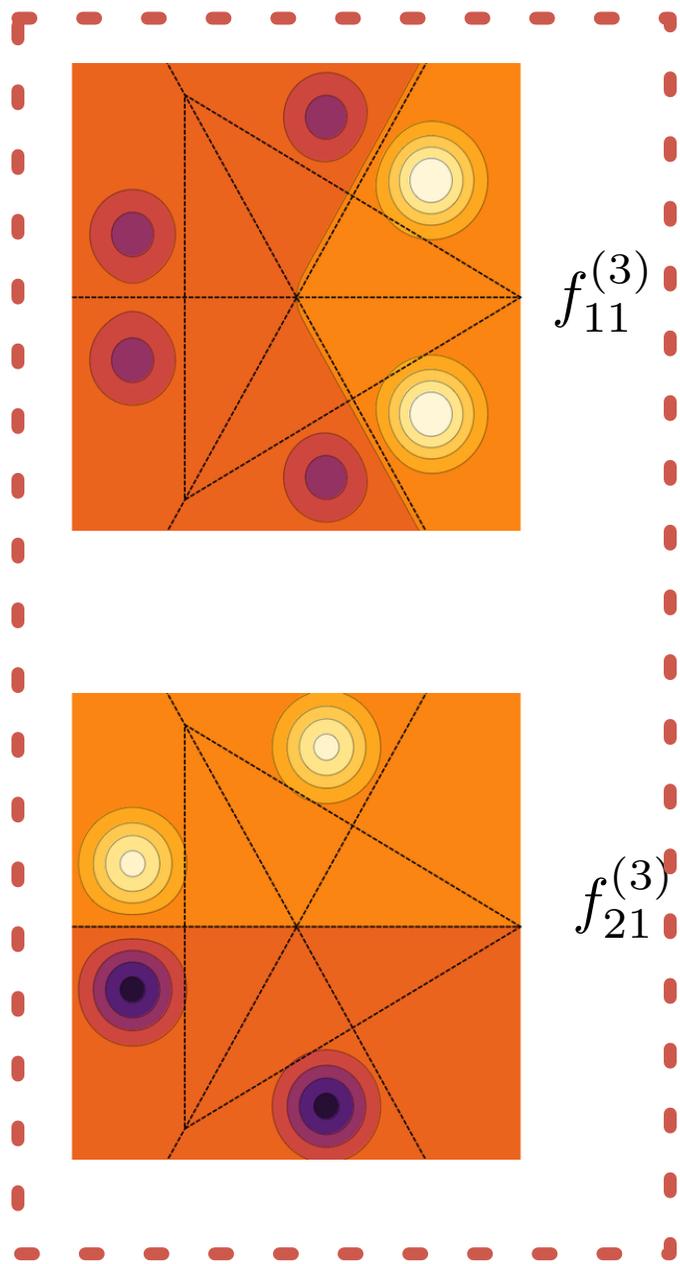
	$r_0$	$r_1$	$r_2$	$s_0$	$s_1$	$s_2$
Identity	1	1	1	1	1	1
Alternate	1	1	1	-1	-1	-1
Matrix	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$
Regular	$\mathbb{1}_{6 \times 6}$	see multiplication table				

We used the circled entries to make  $f_{a1}^{(3)}$

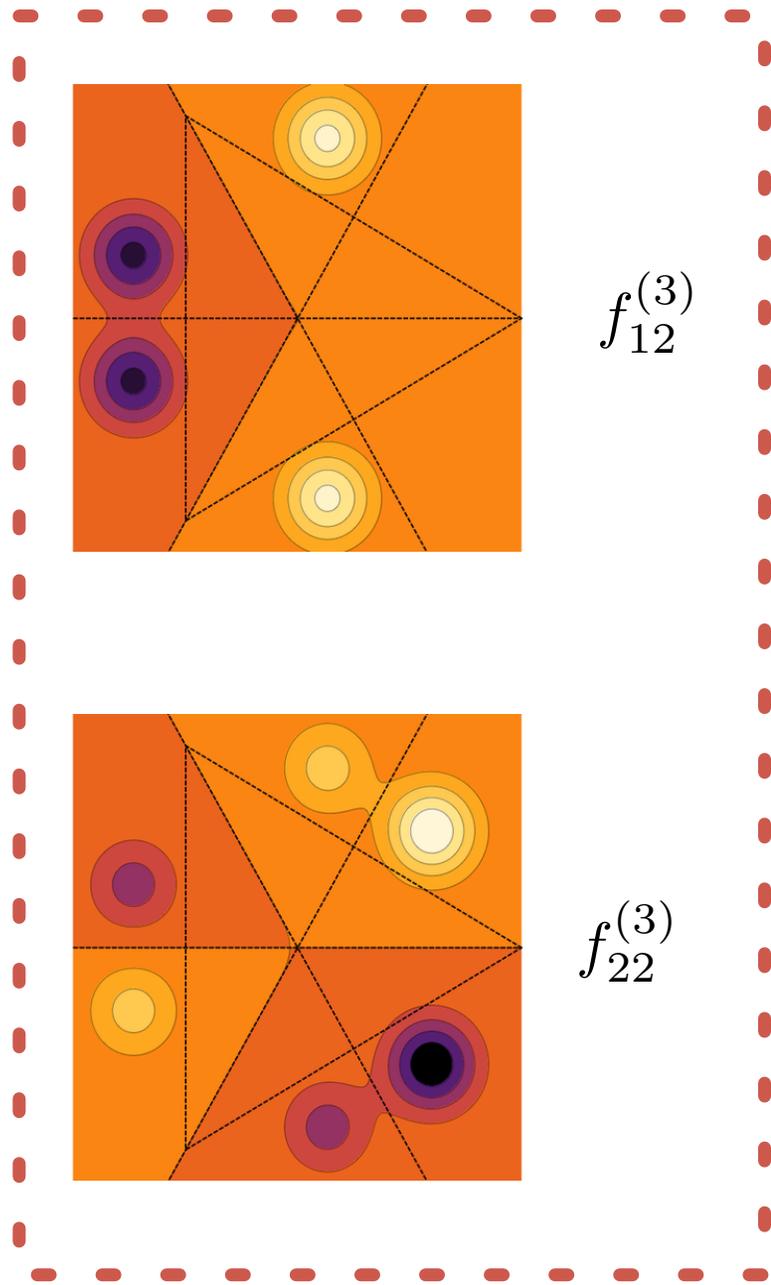
- Here  $\mathbb{1}_{6 \times 6}$  is the  $6 \times 6$  identity matrix. Some matrix representatives of the regular representation are

$$D(r_1) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$$D(s_0) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$



Partners in an irreducible rep



Partners in an irreducible rep

- The functions  $f_{ab}^{(\mu)}$  are partners in a irreducible representation  $(\mu)$ . Take  $b=1$  for example. Being partners means

$$\bigcirc_g f_{ab}^{(\mu)} = f_{cb}^{(\mu)} (D_{ca}^{(\mu)}(g))^*$$

- What this means is that

$$f_{11}^{(3)}$$

can be transformed into  $f_{21}^{(3)}$  by a linear combination of group operations. Indeed

$$f_{21}^{(3)} = \frac{1}{2} O_{r_1} f_{11}^{(3)} - \frac{1}{2} O_{r_2} f_{11}^{(3)}$$

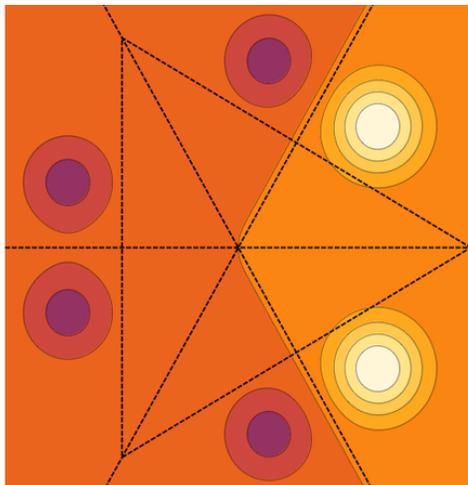
Similarly  $f_{21}^{(\mu)}$  can be transformed to  $f_{11}^{(3)}$ .

- But no amount of group transformations will change  $f_{11}^{(1)}$  to  $f_{11}^{(3)}$ . ( $f_{11}^{(1)}$  is totally symmetric)

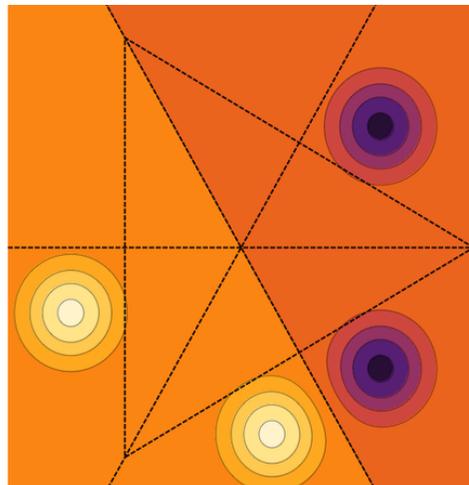
# Partners in the same irrep are mixed by the group operations

(but different irreps do not mix)

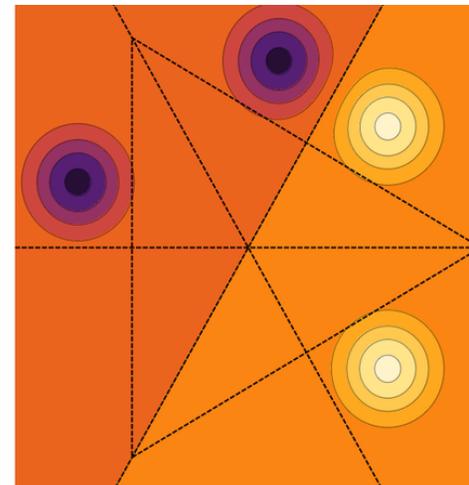
$f_{11}^{(3)}$



$= -1/2$

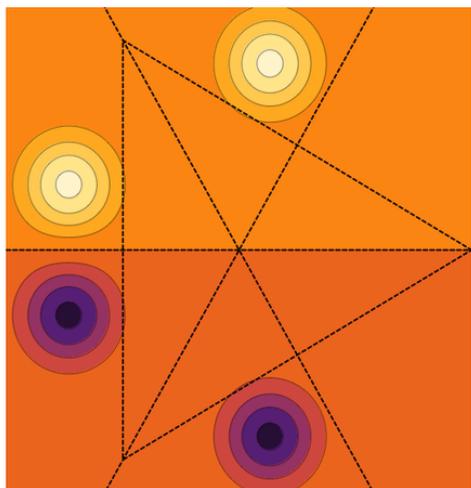


$+ 1/2$

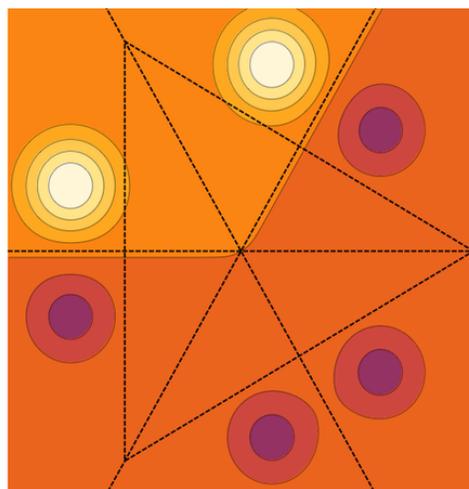


$$f_{11}^{(3)} = \frac{1}{2}(-O_{r_1} + O_{r_2})f_{21}^{(3)}$$

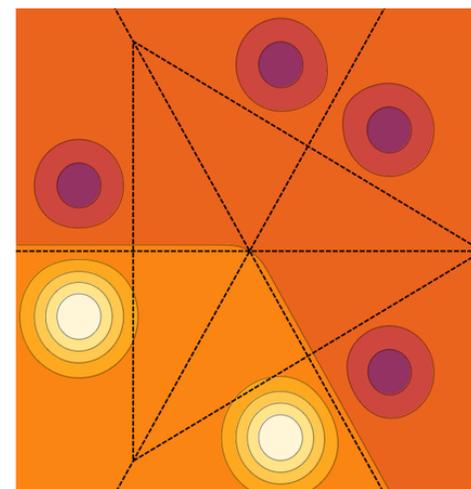
$f_{21}^{(3)}$



$= 1/2$



$- 1/2$



$$f_{21}^{(3)} = \frac{1}{2}(O_{r_1} - O_{r_2})f_{11}^{(3)}$$

• Proof that  $f_{ab}^{(m)}$  are partners in an irrep:

$$O_g f_{ab}^{(m)}(x) = \frac{n_M}{n_G} \sum_{g_1} D_{ba}^{(m)}(g_1^{-1}) O_{g_1} f$$

So

$$O_g f_{ab}^{(m)}(x) = \frac{n_M}{n_G} \sum_{g_1} D_{ba}^{(m)}(g_1^{-1}) O_g O_{g_1} f$$

Now

$$O_{gg_1} = \frac{n_M}{n_G} \sum_{g_1} D_{ba}^{(m)}(g_1^{-1}) O_{gg_1} f$$

• Now as  $g_1$  runs over the group so does  $gg_1 = g_2$   
Define

$$g_2 = gg_1$$

$$g_2^{-1} = g_1^{-1} g^{-1}$$

$$g_2^{-1} g = g_1^{-1}$$

So

$$O_g f_{ab}^{(m)}(x) = \frac{n_M}{n_G} \sum_{g_2} D_{ba}^{(m)}(g_2^{-1} g) O_{g_2} f$$

$$= \frac{n_M}{n_G} \sum_{g_2} D_{bc}^{(m)}(g_2^{-1}) D_{ca}^{(m)}(g) O_{g_2} f(x)$$

$$= \left( \frac{n_M}{n_G} \sum_{g_2} D_{bc}^{(m)}(g_2^{-1}) O_{g_2} f \right) D_{ca}^{(m)}(g)$$

$$O_g f_{ab}^{(m)} = f_{cb}^{(m)} D_{ca}^{(m)}(g)$$

## The Decomposition Into Elements of definite symmetry

• The operators  $\hat{e}_{ab}^{(m)}$  form a complete basis for the group algebra  $\hat{x} = \sum x_i \hat{g}_i$

• This means that any  $\hat{g}_i$  can be expressed as a linear combo of  $\hat{e}_{ab}^{(m)}$ . In particular

$$\mathbb{1} = \sum_{m,a,b} c_{ab}^{(m)} \hat{e}_{ab}^{(m)} \quad \hat{e}_{ab}^{(m)} \equiv \frac{n_m}{n_G} \sum_g (D_{ab}^{(m)}(g))^* \hat{g}$$

Then since  $\langle \hat{e}_{ab}^{(m)}, \hat{e}_{cd}^{(n)} \rangle = \frac{n_m}{n_G} \delta_{mn} \delta_{ac} \delta_{bd}$   
we find

$$\langle \hat{e}_{ab}^{(m)}, \mathbb{1} \rangle = c_{ab}^{(m)} n_m / n_G$$

• Then for any "vector"  $\hat{V} = \sum_i v_i \hat{g}_i$

$$\hat{V} = \sum_g v(g) \hat{g} = \sum_i v(g_i) \hat{g}_i = \sum v_i \hat{g}_i$$

We have

$$\langle \mathbb{1}, \hat{V} \rangle = v(\mathbb{1}) \quad \leftarrow \text{just the component of } \hat{V} \text{ along } \mathbb{1}$$

$$\langle \hat{V}, \mathbb{1} \rangle = v^*(\mathbb{1}) \quad \leftarrow \text{the complex conjugate}$$

Thus

$$C_{ab}^{(m)} = \frac{n_G}{n_\mu} \langle \hat{e}_{ab}^{(m)}, \mathbb{1} \rangle = \frac{n_G}{n_\mu} \left( \frac{n_\mu}{n_G} D_{ab}^{(m)}(\mathbb{1}) \right)$$

component of  $\hat{e}$   
along  $\mathbb{1}$

$$C_{ab}^{(m)} = D_{ab}^{(m)}(\mathbb{1})$$

$$C_{ab}^{(m)} = \delta_{ab}$$

The matrix of  $\mathbb{1}$  ← group op  
is the identity matrix  
 $\mathbb{1}_{ab}^{(m)} = \delta_{ab}$

So

$$\mathbb{1} = \sum_{m,a,b} \delta_{ab} \hat{e}_{ab}^{(m)}$$

$$\mathbb{1} = \sum_m \sum_a \hat{e}_{aa}^{(m)}$$

Then we may decompose any function into components

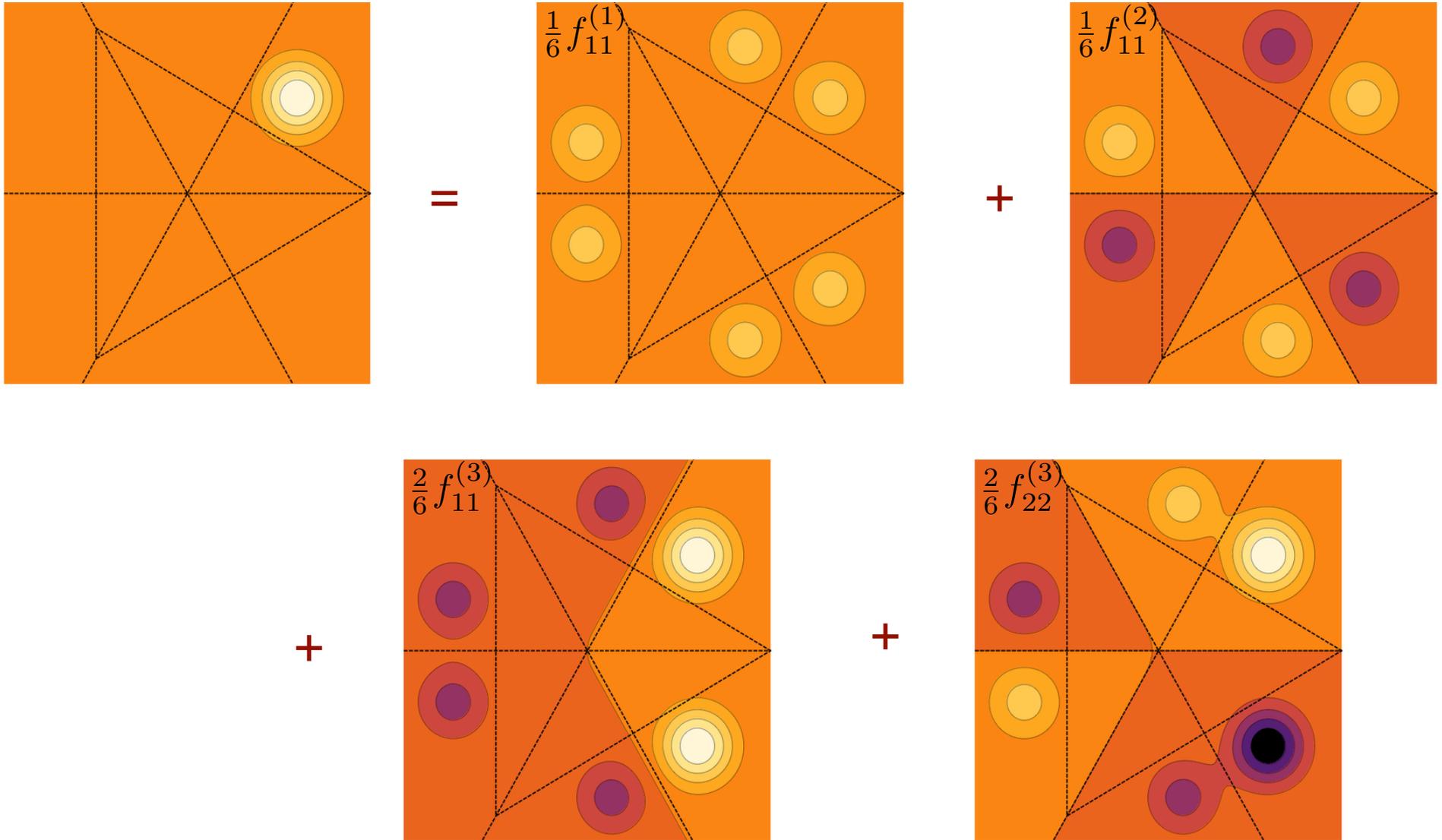
$$f = \mathbb{1} f$$

$$f = \sum_m \sum_a \hat{e}_{aa}^{(m)} f = \sum_m \sum_a f_{aa}^{(m)}$$

- The  $f_{aa}^{(m)}$  transform as a row of an irreducible representation.

This is portrayed graphically on the slide.

# Projection theorem portrayed graphically



$$f = \sum_{\mu, a} f_{aa}^{(\mu)} = f_{11}^{(1)} + f_{11}^{(2)} + f_{11}^{(3)} + f_{22}^{(3)}$$