Groups

Take thee fixed protons arranged in a triangle.

The electron wave functions are very symmetric. There are degeneracies. Group theory can classify how symmetric the wave functions are, and the degeneracy of the eigenstates.

Defining Props

- A group G is a set of elmenets closed under a multiplication rule:

① $\hat{g}_1$ and $\hat{g}_2 \in G$

$$\hat{g}_1 \cdot \hat{g}_2 \in G$$

② The product is associative

$$(\hat{g}_1 \cdot \hat{g}_2)\,\hat{g}_3 = \hat{g}_1(\hat{g}_2\hat{g}_3)$$

But not necessarily commutative $g_1 g_2 \neq g_2 g_1$ in general (though it can happen)

③+④ There is an identinty element and inverse

$$\hat{g} \cdot \hat{e} = \hat{g} \qquad \text{for all } g \in G$$

$$\hat{g}^{-1}\hat{g} = \hat{e} \qquad g^{-1} \in G \text{ when } g \in G$$

Examples:

Z_n the n-roots of unity

Take Z_3:

$$1, \; e^{2\pi i/3}, \; e^{2\pi i 2/3}$$
$$\uparrow \quad \uparrow \quad \uparrow$$
$$g_0, \; g_1, \; g_2$$

- Construct a multiplication table:

	g_0	g_1	g_2
g_0	g	g_1	g_2
g_1	g_1	g_2	g_0
g_2	g_2	g_0	g_1

This group is abelian meaning commutative $\hat{g}_i \cdot \hat{g}_j \equiv \hat{g}_j \cdot \hat{g}_i$

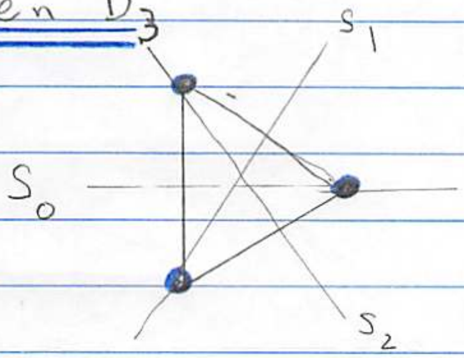
- In general given a set of group elements

$$(g_0, g_1 \cdots g_{n-1})$$

Multiplication by a group element just permutes the elements, e.g.

$$g_1 (g_0, g_1, g_2) \longrightarrow (g_1 \, g_2, g_0)$$

Then D_3



Notation wikipedia

- The set of operations which leave the triangle invariant $\equiv$ Dihedral group D_3

$\hat{r}_0 \equiv$ rotation by $0 \equiv \underline{\mathbb{1}}$

$\hat{r}_1 =$ rotation by $2\pi/3$

$\hat{r}_2 =$ rotation by $2\pi \cdot 2/3$

$\hat{s}_0 =$ reflection over the line S_0

$\hat{s}_1 =$ " " " " S_1

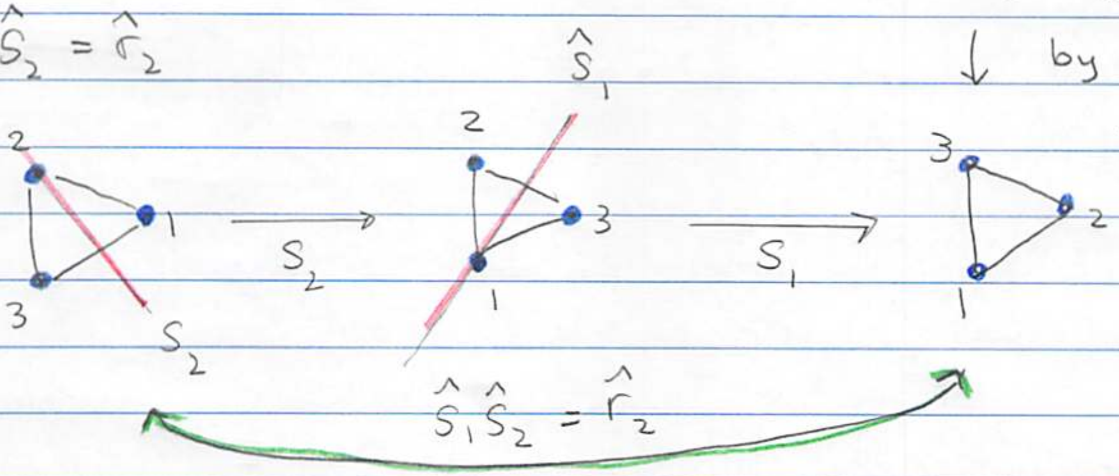
$\hat{s}_2 =$ " " " " S_2

- Lets work at the group multiplication table in this case:

- Look at the operation $s_1 s_2$, s_2 first followed by s_1:

Then lets look at $\hat{S}_1 \cdot \hat{S}_2$:

$\hat{S}_1 \hat{S}_2 = \hat{r}_2$

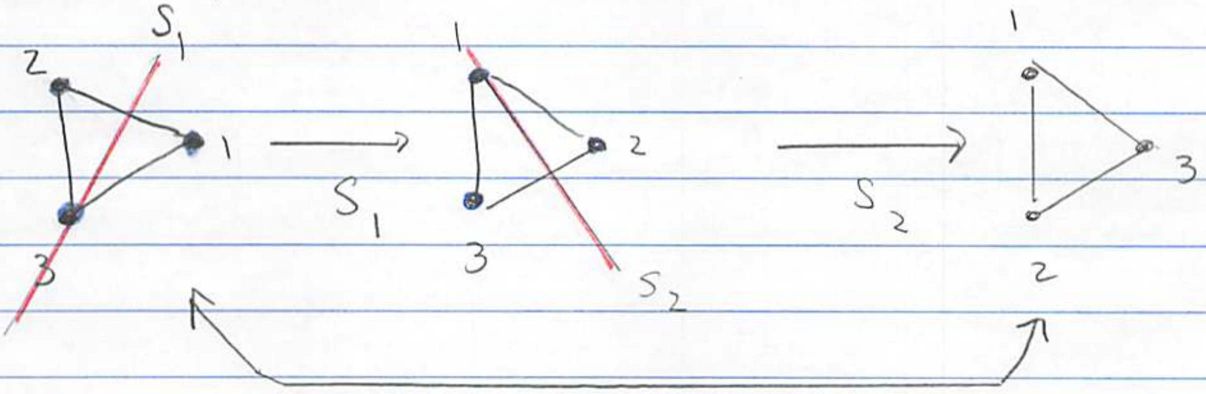


This rotated by $4\pi/3$ relative to the original

- We see that $s_1 s_2$ is a rotation by $4\pi/3$.

Then similarly:

$\hat{S}_2 \hat{S}_1 = \hat{r}_1$



$S_2 S_1 = r_1$ = rotation by $2\pi/3$

- Thus we see that the group is <u>non-abelian</u> since $g_1 g_2 \neq g_2 g_1$ (i.e. $s_1 s_2 \neq s_2 s_1$).

The full group multiplication table is below.

	r_0	**r_1**	**r_2**	**s_0**	**s_1**	**s_2**
r_0	r_0	r_1	r_2	s_0	s_1	s_2
r_1	r_1	r_2	r_0	s_1	s_2	s_0
r_2	r_2	r_0	r_1	s_2	s_0	s_1
s_0	s_0	s_2	s_1	r_0	r_2	r_1
s_1	s_1	s_0	s_2	r_1	r_0	r_2
s_2	s_2	s_1	s_0	r_2	r_1	r_0

Representations

A representation is a homomorphism (aka a many-to-one map) between the group elements and a set of linear operators or matrices $D(g)$

$$g \longrightarrow D(g)$$

Such that

$$e \longrightarrow \mathbb{1} \quad \text{identity maps to unit matrix}$$

$$g_1 g_2 \longrightarrow D(g_1 g_2) = D(g_1) D(g_2)$$

Example 1

- The identity representation. All elements of the group are mapped to the number 1

$$g_1 g_2 \longrightarrow 1 \cdot 1 = 1$$

This is clearly a many-to-one map and is not invertable

Example 2

- Take the space of vectors in 2d $\vec{V} = \begin{pmatrix} V^x \\ V^y \end{pmatrix}$
- We know how to implement reflections and rotations in this space of vectors.

We can use this to represent the group D_3

$$D_3 = \{ r_0, r_1, r_2, s_0, s_1, s_2 \}$$

To write down this representation let us formalize our notion of represention more sharply

Representations (formal version)

- For each group operator g associate a linear operator $\hat{O}_g$ on a vector space $\mathbb{V}$ with an inner product $\langle \, , \rangle$

$$g \longrightarrow \hat{O}_g \qquad g_1 g_2 \rightarrow \hat{O}_{g_1 g_2} = \hat{O}_{g_1} \hat{O}_{g_2}$$

- The matrices are found by specifying a basis of the vector space $\vec{e}_b$:

$$\boxed{\hat{O}_g \circ \vec{e}_a = \vec{e}_b D_{ba}(g)} \qquad \boxed{\langle e_b , \hat{O} e_a \rangle = D_{ba}}$$

note order

- Then a vector $\vec{V} = V_a \vec{e}_a = \vec{e}_a V_a$ is transformed as

$$\hat{O}_g \vec{V} = \hat{O}(g) (V_a \vec{e}_a)$$

$$= (\hat{O}_g \vec{e}_a) V_a$$

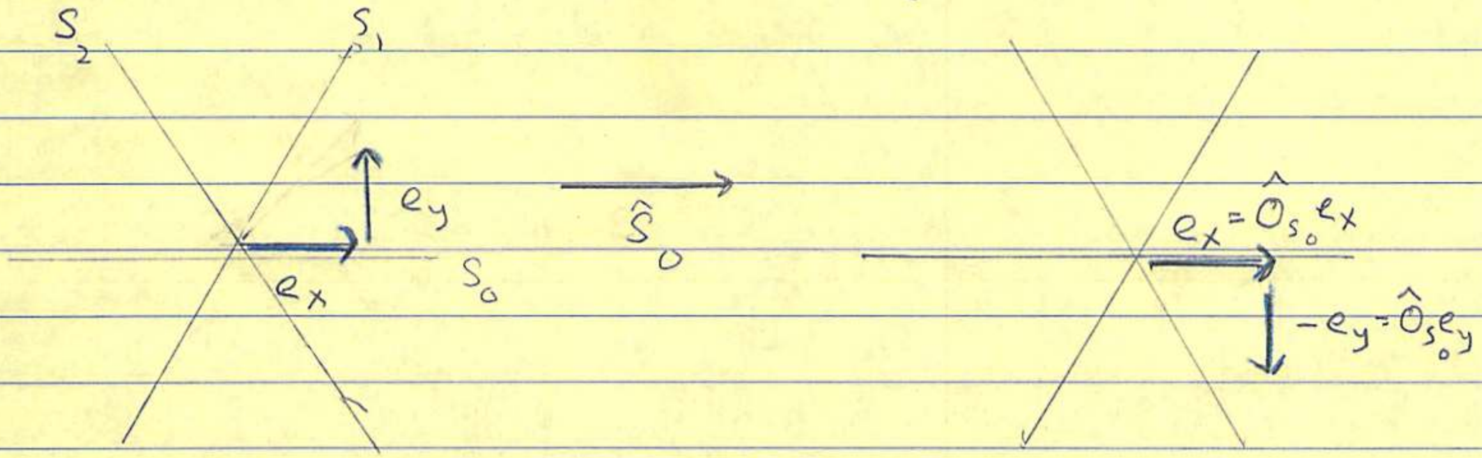
$$O_g V = \vec{e}_b D^{(g)}_{ba} V_a$$

- The $\vec{e}_b$ are known as partners in the representation

i.e.

$$V_g \xrightarrow[g]{} \underline{V}_b = D_{ba}(g) V_a$$

- Then take vectors under $\hat{S}_0$

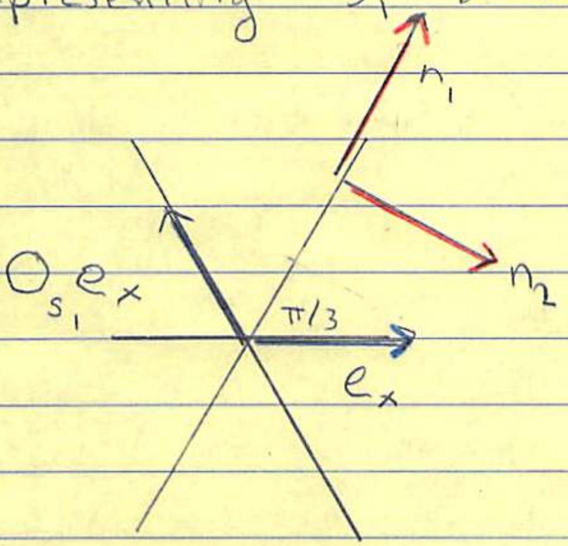


$$O_{s_0} \vec{e}_x = \vec{e}_x$$
$$O_{s_0} \vec{e}_y = -\vec{e}_y$$

or $O_{s_0} \vec{e}_a = \vec{e}_b \, D^b{}_a(s_0)$

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

- Similary we can find a matrix representing s_1. Look at $\vec{n}_1, \vec{n}_2$ and $\vec{e}_x$ (unit vects)



$$\vec{e}_x = \cos\pi/3 \, \vec{n}_1 + \sin\pi/3 \, \vec{n}_2$$

$$O_{s_1} e_x = \cos\pi/3 \, \vec{n}_1 - \sin\pi/3 \, \vec{n}_2$$

$$\vec{n}_1 = \cos\pi/3 \, \vec{e}_x + \sin\pi/3 \, \hat{e}_y$$

$$\vec{n}_2 = \sin\pi/3 \, \vec{e}_x - \cos\pi/3 \, \hat{e}_y$$

So some algebra shows

$$O_{s_1} e_x = \cos(2\pi/3) \, \vec{e}_x + \sin(2\pi/3) \, \vec{e}_y$$
$$= -1/2 \, \vec{e}_x + \sqrt{3}/2 \, \vec{e}_y$$

Then similary one can show

$$O_{s_1} e_y = \overbrace{\sin(2\pi/3)}^{+\sqrt{3}/2} e_x \overbrace{- \cos(2\pi/3)}^{-(-1/2)} e_y$$

And thus

$$O_{s_1} \vec{e}_a = \vec{e}_b \, D_{ba}(g) \quad \text{with}$$

$$D(s_1) = \begin{pmatrix} \cos(2\pi/3) & \sin(2\pi/3) \\ \sin(2\pi/3) & -\cos(2\pi/3) \end{pmatrix} = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix}$$

The remaining matrices are then

$$D(r_0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$D(r_1) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \quad \text{with} \quad \theta = 2\pi/3$$

$$D(r_1) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$D(r_2) = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} \quad \text{rotations by } 4\pi/3$$

$$D(s_0) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad D(s_1) = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix} \qquad D(s_2) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix}$$

- This representation is **faithful**, meaning that each group element is associated with a unique matrix

Example 2.5 the alternating representation of D_3

Notice (by examining the multiplication table)

reflection x rotation = reflection

reflection x reflection = rotation

rotation x rotation = rotation

So lets associatie reflections with the number -1, and the rotations with the number 1

Element	r_0	r_1	r_2	s_0	s_1	s_2
Identity Rep	1	1	1	1	1	1
Alternating Rep	1	1	1	-1	-1	-1
Matrix Rep	see previous page this is faithful					

these are not faithful

See next page

D_3 Matrix Representation Summary

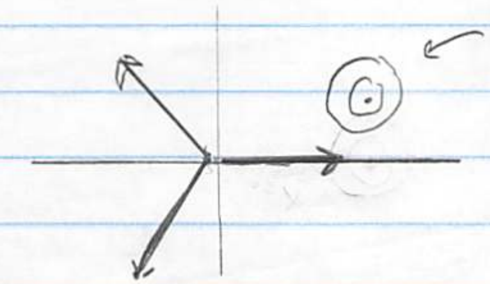
	r_0	r_1	r_2	s_0	s_1	s_2
Identity	1	1	1	1	1	1
Alternate	1	1	1	-1	-1	-1
Matrix	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2}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

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

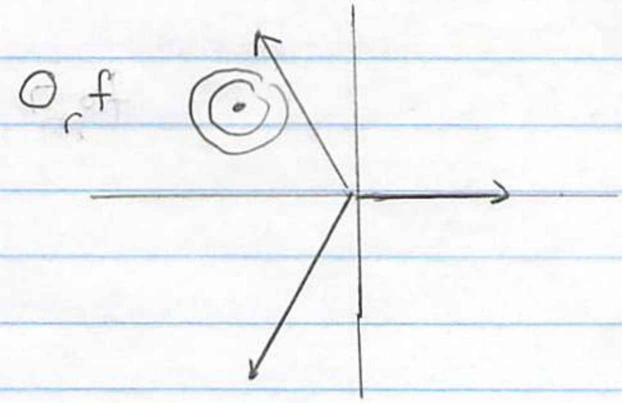
$$D(r_1) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \qquad D(s_0) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Representation of D_3 in the space of functions

Take a function $f(\vec{x}) = e^{-(x-x_0)^2-(y-y_0)^2}$, $\vec{x} \equiv (x,y)$


contours of $f(x,y) = f(\vec{x})$

The group elements should transform the function. For instance $r \equiv$ rotation by $2\pi/3 \equiv r_1$ should rotate f_G



Clearly

$$(O_r f)(x') = f(x)$$

where $\vec{x}' = r\vec{x}$ are the rotated coordinates. Thus since $\vec{x} = r^{-1}\vec{x}'$

$$(O_r f)(x') = f(r^{-1}x')$$

But, x' is just a dummy arguement on both sides

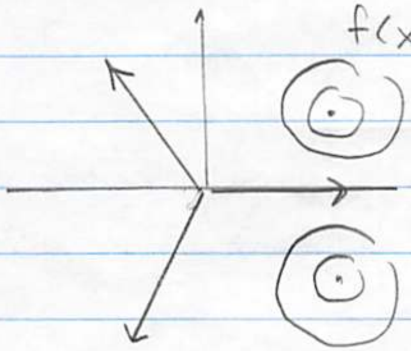
$$(O_r f)(\vec{x}) = f(r^{-1}\vec{x})$$

In general

$$\boxed{(O_g f)(x) = f(g^{-1}x)}$$

e.g. for $S_0 \equiv$ reflection over x-axis

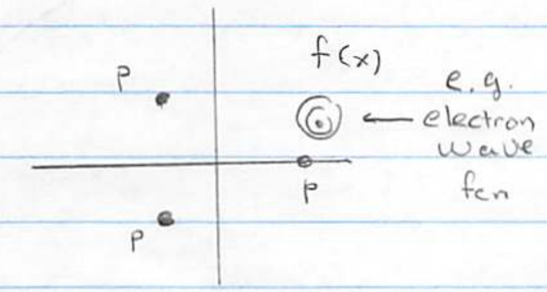
$(O_{S_0} f)(x,y) = f(-x,y)$

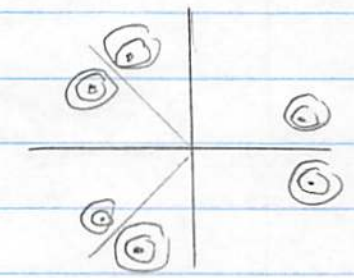


- The operators $\overset{\swarrow \text{identity}}{O_{r_0}}, O_{r_1}, O_{r_2}, O_{s_0}, O_{s_1}, O_{s_2}$ give a faithful representation of the group D_3 in the Hilbert space

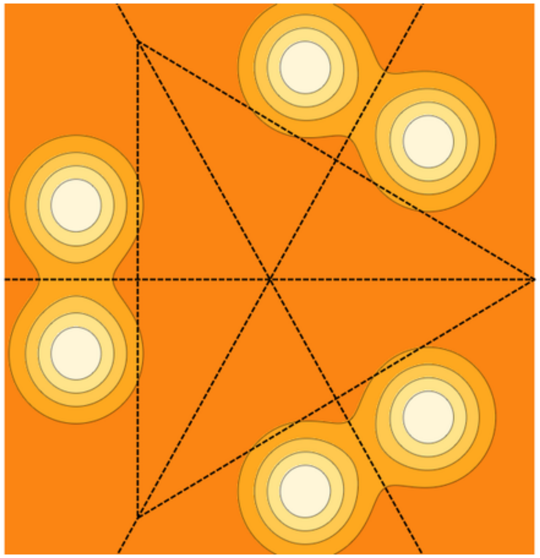
- Note we can construct a highly symmetric function by averaging over the group operations

$$f_S(\vec{x}) = \frac{1}{6} \sum_g O_g f(\vec{x})$$

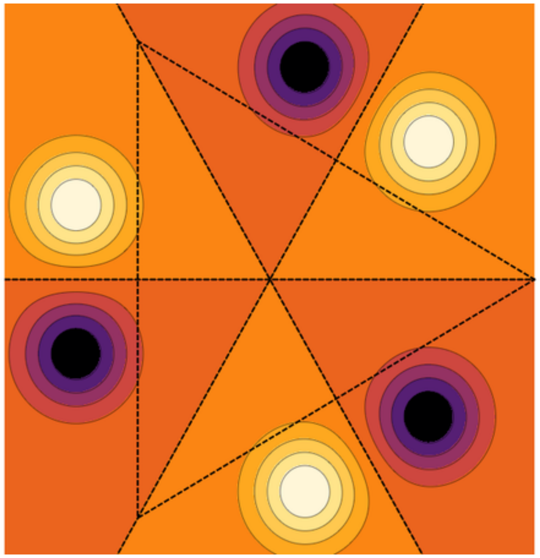




$f_S(\vec{x})$ is invariant under all the operations of the group



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



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

- Then we prove that $f_s(x)$ is invariant as follows:

$$O_{g'} f_s = \frac{1}{6}\sum_{g} O_{g'} O_g f(x)$$

$$g'' = g'g$$

$$= \frac{1}{6}\sum_{g} O_{g'g} f(x) \xrightarrow{\quad} = \frac{1}{6}\sum_{g''} O_{g''} f(x) = f_s(x)$$

Here multiplication by g' just rearranges the sum

$$g' \cdot \{ g_0, g_1, g_2 \cdots\cdots \}$$

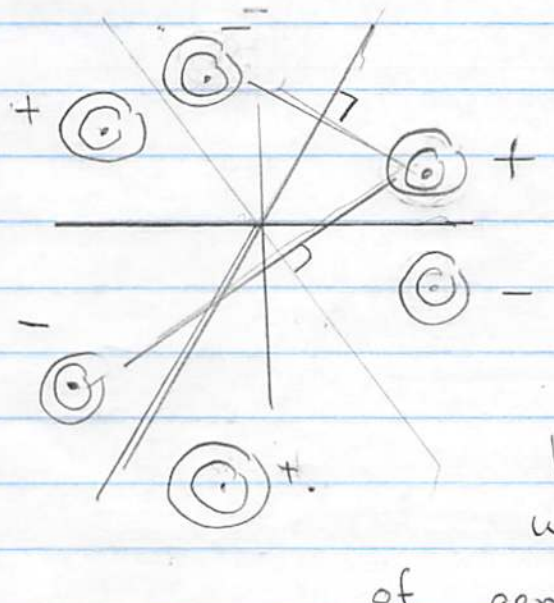
$$= \{ \text{a rearrangement of } g_0, g_1, g_2 \ldots \}$$

$$\sum_{g} O_{g'g} = \sum_{g''} O_{g''}$$

$$g'' \equiv g'g$$

- We have associated + with rotations and − with reflections. Let us construct in the alternating rep

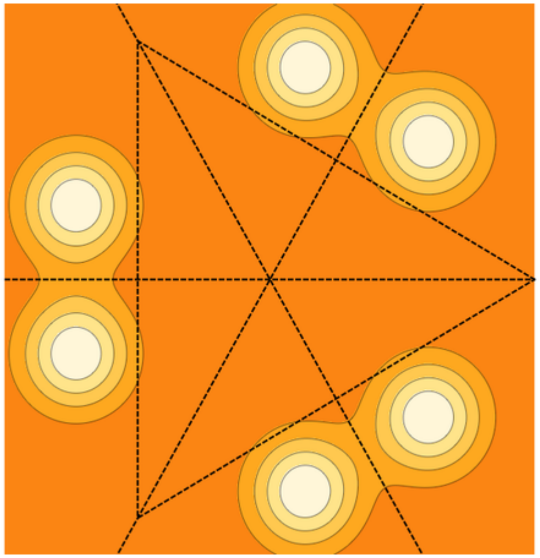
$$f_A(x) = \frac{1}{6}\left(O_{r_0}f + O_{r_1}f + O_{r_2}f - O_{s_0}f - O_{s_1}f - O_{s_2}f\right)$$



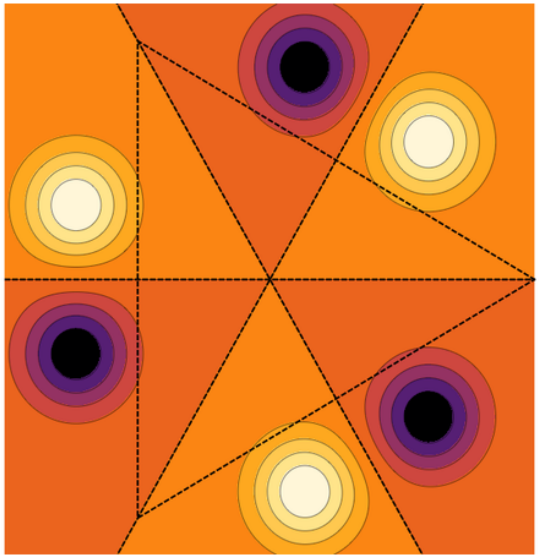
Clearly

$$\int d^2x\, f_A(\vec{x})\, f_S(x) = 0$$

This function is also highly symmetric. We will generalize this procedure of generating symmetric functions later



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



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

The Regular Representation

- Consider the group elements themselves $\hat{g}_1, \hat{g}_2, \hat{g}_3$ as the basis vectors of a vector space of operators

$$\hat{x} = \overset{\substack{\text{number}\\ \downarrow}}{x_1}\,\underset{\nwarrow\ \text{ops}}{\hat{g}_1} + x_2\hat{g}_2 + x_3\hat{g}_3$$

- Then multiptication by the group element $\hat{g}$ defines a linear map (i.e. a matrix rep of $\hat{g}$) in the vector space of ops

$$\hat{g}\hat{x} = x_1\hat{g}\hat{g}_1 + x_2\hat{g}\hat{g}_2 + x_3\hat{g}\hat{g}_3$$

- Take Z_3 and its multiplication table. Take g_1 for example

	g_0	g_1	g_2
g_0	g_0	g_1	g_2
g_1	g_1	g_2	g_0
g_2	g_2	g_0	g_1

$$\hat{g}_1\hat{g}_0 = 0 + \hat{g}_1 + 0$$

$$\hat{g}_1\hat{g}_1 = 0 + 0 + \hat{g}_2$$

$$g_1\hat{g}_2 = \hat{g}_0 + 0 + 0$$

just read of coefficents

Then

$$D(g_1) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

If we write the "vector" $\hat{x}$

$$\hat{x} = \sum_i x_i \hat{g}_i$$

Then

$$\hat{g}_1 \hat{x} = \hat{g}_i D_{ij}(g_1) x_j$$

i.e.

$$x_i \xrightarrow[\hat{g}_1]{} D_{ij}(g_1) x_j$$

Similarly we record

$$D(g_0) = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \qquad D(g_2) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

Excercise write down the regular representation for D_3. A number of elements are shown on the following page

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 multiplacation table		

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

$$D(r_1) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \qquad D(s_0) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$