

Lect 5: Character tables for finite groups

①

* General guidance

$$\textcircled{1} \sum_j m_j^2 = |G|$$

$$\textcircled{2} \sum_j 1 = n_c$$

$$\textcircled{3} \sum_{\alpha=1}^{n_c} n_{\alpha} \chi_i^*(C_{\alpha}) \chi_j(C_{\alpha}) = |G|$$

$$\textcircled{4} \sum_j \chi_j^*[C_{\alpha}] \chi_j[C_{\beta}] = \frac{|G|}{|n_{\alpha}|} \delta_{\alpha\beta}$$

where j is the index for irreducible Reps, n_c is # of classes,

n_{α} is the # of elements in class C_{α} , $|G|$ is the order of group.

* Other properties

① any group has the identity Rep.

② Any irreducible representations of the quotient group is also an irreducible Rep of the original group. — looking for invariant subgroups.

③ If G has irreducible ~~complex~~ complex representations, it's characters must have complex values. Then its complex conjugation is also a non-equivalent irreducible Rep.

④ For group G , it's 1D irreducible representation multiplied by any other irreducible representation is also an irreducible representation.

⑤ The irreducible representation for the group G is also a representation of its subgroup H . But it is often reducible.

Nevertheless, the possibility of reducing is often limited.

⑥ If $G = H_1 \otimes H_2$, then the irreducible representations of G can be represented as irreducible representations of H_1 and H_2 .
 direct product of

* Cyclic group.

$$C_N = \{E, R, R^2, \dots, R^{N-1}\}, R^N = E$$

N irreducible 1D representations. The j -th representation

$$D^j(R) = e^{-i2\pi j/N} \quad \text{for } 0 \leq j \leq N-1$$

and hence $D^j(R^m) = e^{-i2\pi mj/N} \quad \text{for } 0 \leq m \leq N-1$

	E	R
A	1	1
B	1	-1

C_2

	E	R	R^2
A	1	1	1
E	1	ω	ω^2
E'	1	ω^2	ω

C_3

m
 0 $\omega = e^{-i2\pi/3}$
 1 discrete angular momentum
 -1

	E	R	R^2	R^3
A	1	1	1	1
B	1	-1	1	-1
E	1	-i	-1	i
E'	1	i	-1	-i

C_4

	E	R^2	R^4	R^3	R^5	R
A	1	1	1	1	1	1
B	1	1	1	-1	-1	-1
E ₁	1	ω	ω^2	-1	$-\omega$	$-\omega^2$
E ₂	1	ω^2	ω	1	ω^2	ω
E' ₁	1	ω^2	ω	-1	$-\omega^2$	$-\omega$
E' ₂	1	ω	ω^2	1	ω	ω^2

$C_6 = C_3 \otimes C_2 = \{E, R, R^2\} \otimes \{E, R^3\}$

Question: How many complex Reprs and real Reprs?

Answer: Consider a class. If for every element g in the class, then g^{-1} is also in this class, then it's called self-inverse class.

The # of self-conjugate (real and pseudo-real) representations equals the # of self-inverse classes, and the # of complex representations equals the # of non self-inverse classes.

For C_4 and C_6 , rotation 180° is a self-inverse operation also forming a class. Including the identity, they have two real representations. For odd order cyclic groups, they only have the identity Rep as a real one.

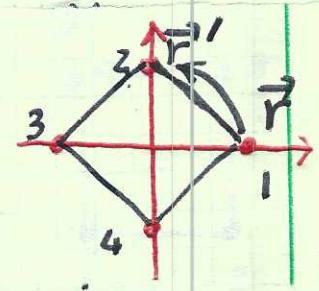
★ Application: QM — molecular orbit

① Symmetry operation on QM wave functions

Consider a symmetry operation g , its operation on space

coordinate: $\vec{r}' = g\vec{r}$.

For example, g : rotation $\frac{\pi}{2}$.



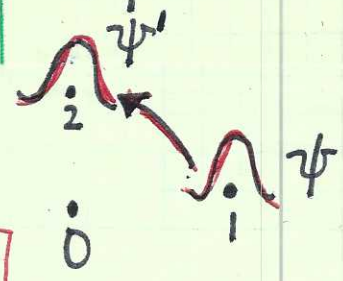
How does it apply to a scalar wavefunction

$\psi(\vec{r})$?

Denote the state after operation $\psi' = g\psi$. We want

~~$\psi(\vec{r})$~~ $\psi'(\vec{r}') = \psi(\vec{r})$

$\psi'(g\vec{r}) = \psi(\vec{r})$
 \Rightarrow $\psi'(\vec{r}) = \psi(g^{-1}\vec{r})$



in the Dirac notation $|1\rangle \leftrightarrow \delta(r-r_1)$, $|2\rangle \leftrightarrow \delta(r-r_2)$ (4)

$$g|1\rangle \rightarrow |2\rangle \Leftrightarrow \delta(r-r_2) = \delta(g^{-1}r-r_1) \leftarrow \text{check: if } r=r_2 \text{ then } g^{-1}r_2=r_1 \checkmark.$$

Now suppose on each point (atom), there exist an atomic orbital $|i\rangle$, then the four orbits form a representation of C_4 . Under this set of basis, we have the matrices of E, R, R^2, R^3

$$E: \begin{matrix} |1\rangle & |2\rangle & |3\rangle & |4\rangle \\ \begin{pmatrix} \langle 1| \\ \langle 2| \\ \langle 3| \\ \langle 4| \end{pmatrix} \end{matrix} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \quad R: \begin{matrix} |1\rangle & |2\rangle & |3\rangle & |4\rangle \\ \begin{pmatrix} \langle 1| \\ \langle 2| \\ \langle 3| \\ \langle 4| \end{pmatrix} \end{matrix} \begin{pmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ & & & 1 \end{pmatrix}, \quad R^2: \begin{pmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ & & & 1 \end{pmatrix}, \quad R^3: \dots$$

hence $\chi(E) = 4, \chi(R) = \chi(R^2) = 0$ (with $\chi(R^3)$ also indicated)

Now we can use the character table of C_4 to decompose this representation into irreducible ones as

$$\# \text{ of } A: \frac{1}{4} \sum_g \chi_A^*(g) \chi(g) = \frac{1}{4} \cdot 4 = 1$$

$$\# \text{ of } B, E, E' = \frac{1}{4} \cdot 4 \cdot 1 = 1$$

$$\Rightarrow A \oplus B \oplus E \oplus E'$$

Let us form the orbits belonging to A, B, E and E' Reps.

$$|\psi_A\rangle = \frac{1}{\sqrt{2}} [|1\rangle + |2\rangle + |3\rangle + |4\rangle] \quad \text{S-wave}$$

$$|\psi_B\rangle = \frac{1}{\sqrt{2}} [|1\rangle - |2\rangle + |3\rangle - |4\rangle] \quad \text{d-wave} \quad m=2$$

$$|\psi_E\rangle = \frac{1}{\sqrt{2}} [|1\rangle + i|2\rangle - |3\rangle - i|4\rangle] \quad \left. \begin{array}{l} \text{p-wave} \\ m=1 \end{array} \right\}$$

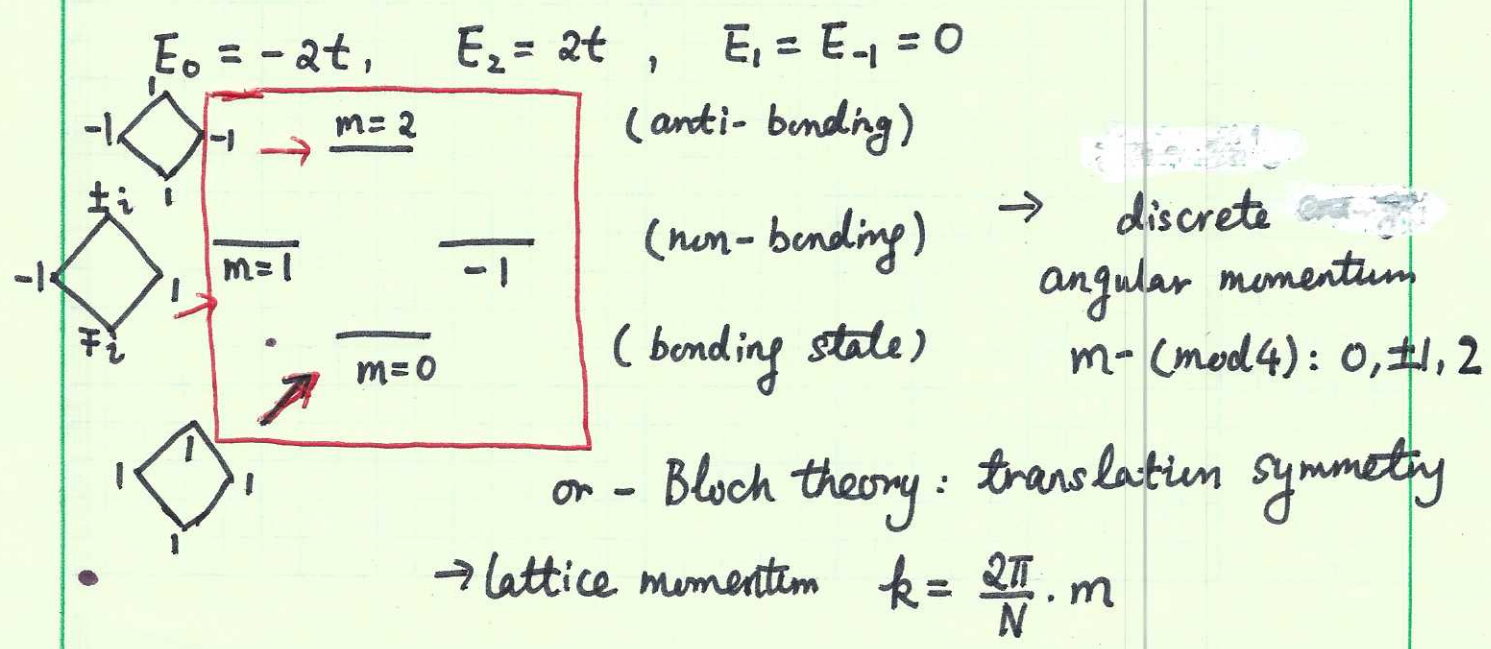
$$|\psi_{E'}\rangle = \frac{1}{\sqrt{2}} [|1\rangle - i|2\rangle - |3\rangle + i|4\rangle] \quad \left. \begin{array}{l} \text{p-wave} \\ m=-1 \end{array} \right\}$$

Compare with the angular momentum eigenstate $\frac{1}{\sqrt{2\pi}} e^{im\theta}$ with $\theta = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2} \leftrightarrow |1\rangle, |2\rangle, |3\rangle, |4\rangle$, we have $m = 0, 2, \pm 1$ for $|\psi_A\rangle, |\psi_B\rangle, |\psi_{E,E'}\rangle$, respectively. We can also check their characters

For example $\left\{ \begin{array}{l} R|\psi_E\rangle = \frac{1}{\sqrt{2}} [|2\rangle + i|3\rangle - |4\rangle - i|1\rangle] = \frac{-i}{\sqrt{2}} [|1\rangle + i|2\rangle - |3\rangle - i|4\rangle] = -i|\psi_E\rangle \\ R|\psi_{E'}\rangle = \frac{1}{\sqrt{2}} [|2\rangle - i|3\rangle - |4\rangle + i|1\rangle] = i|\psi_{E'}\rangle \end{array} \right.$

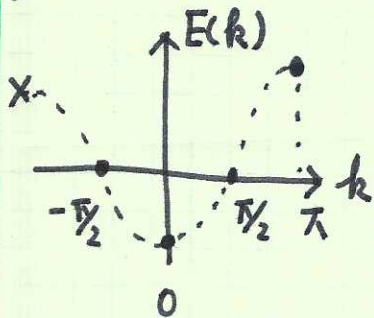
Hence, even we have not given a Hamiltonian, we have already solved the eigenfunctions!

Now consider $H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.)$, plug in the above eigen wavefunctions, we have $E_m = -2t \cos\left(\frac{2\pi}{N} \cdot m\right)$ with $N=4$



$$\psi(r) = \frac{1}{\sqrt{N}} e^{i k \cdot R_i} \dots N=4$$

for 1d lattice, \rightarrow translation with periodical boundary condition



\leftarrow band structure

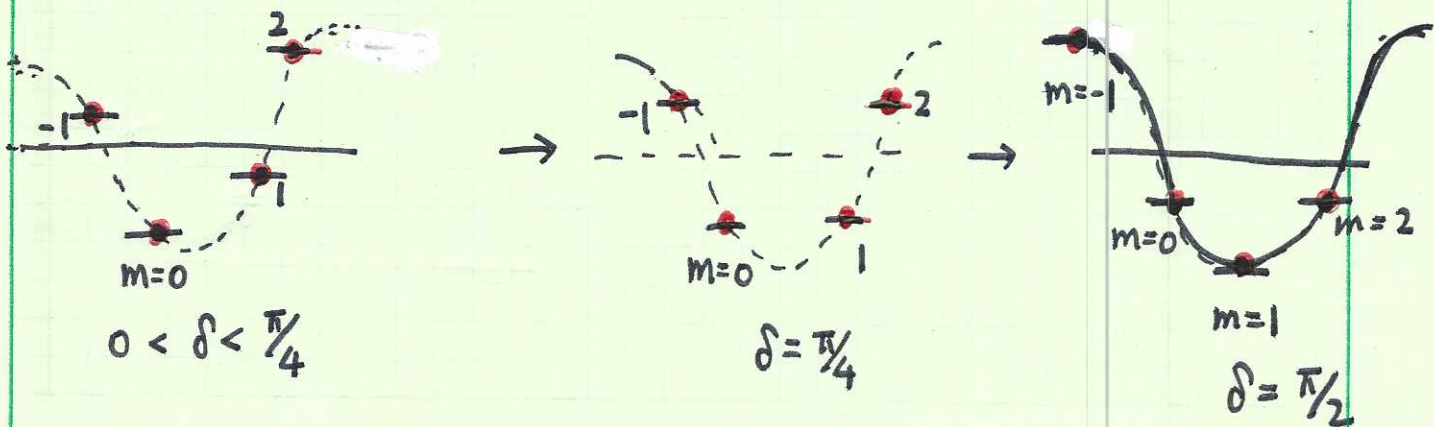
as increasing $N \rightarrow \infty$, molecule becomes crystal, and bond \rightarrow band.

Question: we have seen there exist a degeneracy between $|\psi_E\rangle$ and $|\psi_{E'}\rangle$. For an Abelian group, typically we don't expect degeneracy, since each representation is 1D, and different states don't transform into each other under symmetry operations. Indeed, if we put a flux ϕ into the plaquette, it does not change the C_4 symmetry. The

$$H = -t \sum [c_{i+1}^\dagger c_i e^{i\delta} + h.c.] \text{ with } \frac{\phi}{4} = \delta$$

then the $|\psi_{A,B,E,E'}\rangle$ remain unchanged. But their energies

$$E_m = -2t \cos\left(\frac{2\pi}{N} m - \delta\right)$$



In order to explain the degeneracy pattern at $\delta=0$, we need a higher $\textcircled{7}$ symmetry D_4 .

$\textcircled{8}$ The dihedral group

D_N group is the symmetry group of regular N -polygons. The z -axis is the N -fold axis. The C_N -group is an invariant subgroup, and quotient group is C_2 . In the xy -plane, there are evenly distributed N two-fold axes. D_{2N+1} and D_{2N} have different structures, and we study separately.

$\textcircled{1}$ D_{2N+1} . All the $2N+1$ two-fold axes are equivalent forming one class. For the z -axis, since rotations around $\pm \hat{z}$ axis can be related by the in-plane 2-fold rotation, $R_z(\frac{\pm i}{2N+1} 2\pi)$ belong to the same class. Hence, the C_{2N+1} subgroup contains $n+1$ classes. In total there are $n+2$ classes, and then $n+2$ irreducible representations

$$\sum_{j=1}^{n+2} m_j^2 = 4n+2 \Rightarrow \underbrace{1^2 + 1^2 + 2^2 + \dots + 2^2}_{n} = 4n+2$$

D_{2N+1} must have two non-equivalent 1D representations, corresponding to quotient group C_2 , denoted as A_1 (identity) and A_2 . The

character table has the following structure

	E	$2C_{2n+1}^1$...	$(2n+1)C_2^1$
A_1	1	1	1	1
A_2	1	1	1	-1
E	2	?

(a) look at the class of $2n+1$ two-fold axes, the characters

$$\sum_j |\chi_j(C_2')|^2 = \frac{|G|}{n_{C_2'}} = 2.$$

Since $\chi_{A_1}(C_2') = 1$, and $\chi_{A_2}(C_2') = -1$, $\Rightarrow \chi_E(C_2') = 0$ for all the other 2D representations.

(b) All the classes in D_{2n+1} are self-inverse classes, hence all representations are self-conjugate, (actually real to be checked later!). The characters should be real.

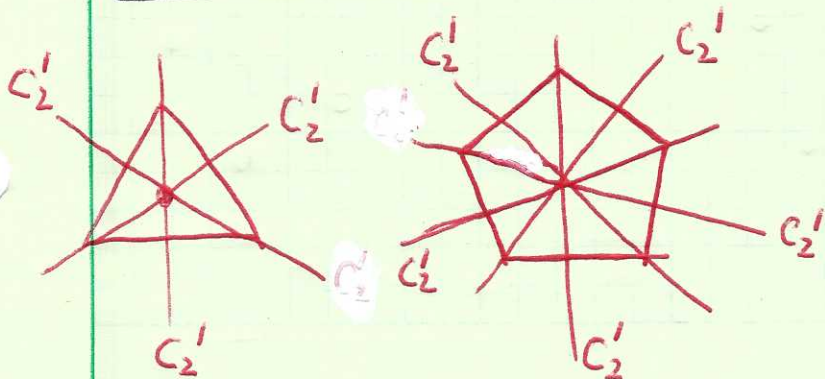
(c) Each 2D representations should be decomposed into a pair of 1D representations. Hence, it should be decomposed into a pair of complex conjugation representations. \Rightarrow

$$\chi_{E_j}(E) = 2, \quad \chi_{E_j}(C_{2n+1}^m) = 2 \cos \frac{2jm\pi}{2n+1}, \quad \chi_{E_j}(C_2') = 0.$$

two examples D_3 and D_5

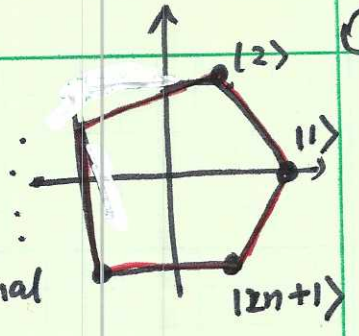
D_3	E	$2C_3$	$3C_2'$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

D_5	E	$2C_5$	$2C_5^2$	$5C_2'$
A_1	1	1	1	1
A_2	1	1	1	-1
E_1	2	p	$-p^{-1}$	0
E_2	2	$-p^{-1}$	p	0



$$\text{where } p = 2 \cos \frac{2\pi}{5} = \frac{\sqrt{5}-1}{2}$$

$$p^{-1} = -2 \cos \frac{4\pi}{5} = \frac{\sqrt{5}+1}{2}$$



Now we use QM states to represent D_{2n+1} group.

Consider states $|1\rangle, |2\rangle, \dots, |2n+1\rangle$ at sites of a regular polygon. They form a $2n+1$ dimensional representation.

The rotation of C_{2n+1} operation: no-fixed sites $\Rightarrow \chi(C_{2n+1}') = 0$.

The 2-fold rotation has a fixed point, $\Rightarrow \chi(C_2') = 1$. Hence, we have

	E	$2C_{2n+1}'$...	$2C_{2n+1}''$	$\overset{2n+1}{C_2'}$
χ	$2n+1$	0	0	0	1

of A_1 : $\frac{1}{|G|} \sum_g \chi_{A_1}^* \chi = \frac{1}{4n+2} (2n+1 + 2n+1) = 1$

A_2 : $\frac{1}{|G|} \sum_g \chi_{A_2}^* \chi = \frac{1}{4n+2} (2n+1 - (2n+1)) = 0$

E_m : $\frac{1}{|G|} \sum_g \chi_{E_m}^* \chi = \frac{1}{4n+2} (4n+2) = 1$

Hence $\chi = A_1 \oplus E_1 \oplus \dots \oplus E_m$ $\leftarrow E_{1 \sim m}$ are 2-dimensional at reps \Rightarrow 2-fold degeneracy.

$|\psi_{A_1}\rangle = \frac{1}{\sqrt{2n+1}} \sum_{i=1}^{2n+1} |i\rangle$

For E_1 , it include the basis with (discrete) angular momentum ± 1

$|\psi_{+}^{E_1}\rangle = \frac{1}{\sqrt{2n+1}} \sum_{j=1}^{2n+1} e^{-i \frac{2\pi}{2n+1} (j-1)} |j\rangle$

$|\psi_{-}^{E_1}\rangle = \frac{1}{\sqrt{2n+1}} \sum_{j=1}^{2n+1} e^{i \frac{2\pi}{2n+1} (j-1)} |j\rangle$

under this basis, we have: the cyclic rotations C_{2n+1}' is diagonal

$\Rightarrow \begin{bmatrix} e^{-i \frac{2\pi}{2n+1} l} & 0 \\ 0 & e^{i \frac{2\pi}{2n+1} l} \end{bmatrix}$

The 2-fold rotation: $C_2' \rightarrow$ Rotation around x-axis

$$C_2'(\hat{x}) : |1\rangle \rightarrow |1\rangle, |2\rangle \leftrightarrow |2n+1\rangle, \dots |n+1\rangle \leftrightarrow |n+2\rangle$$

$$\Rightarrow C_2'(\hat{x}) |\psi_+^{E_1}\rangle = \frac{1}{\sqrt{2n+1}} \sum_{j=1}^{2n+1} e^{-i \frac{2\pi}{2n+1} (j-1)} |2n+3-j\rangle \left\{ \begin{array}{l} j' = 2n+3-j \\ j = 2n+3-j' \end{array} \right.$$

$$= \frac{1}{\sqrt{2n+1}} \sum_{j'=1}^{2n+1} e^{-i \frac{2\pi}{2n+1} (2n+2-j')} |j'\rangle = \frac{1}{\sqrt{2n+1}} \sum_{j'=1}^{2n+1} e^{i \frac{2\pi}{2n+1} (j'-1)} |j'\rangle$$

$$= |\psi_-^{E_1}\rangle$$

Similarly $C_2'(\hat{x}) |\psi_{1-}^{E_1}\rangle = |\psi_+^{E_1}\rangle \Rightarrow C_2'(\hat{x}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

How about other C_2' , — axis at angle $\frac{2\pi}{2n+1}$?

Consider the similar transformation of a rotation

$$R' = R R_{\hat{n}}(\theta) R^{-1} \text{ — check the direction } \hat{n}' = R\hat{n}$$

then $R'\hat{n}' = R \cdot R_{\hat{n}}(\theta) R^{-1} R\hat{n} = R\hat{n} = \hat{n}'$, hence the rotation axis changes to

Hence the representation matrix for the C_2 with axis at

the angle of φ is

$$\begin{pmatrix} e^{-i\varphi} & 0 \\ 0 & e^{i\varphi} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{i\varphi} & \\ & e^{-i\varphi} \end{pmatrix} = \begin{pmatrix} 0 & e^{-i2\varphi} \\ e^{i2\varphi} & 0 \end{pmatrix}$$

in Summary E_1 -rep For C_{2n+1} rotation: \rightarrow

C_2 around axis

at $\frac{2\pi}{2n+1} l$ -angle \rightarrow

$$\begin{pmatrix} e^{-i \frac{2\pi}{2n+1} l} & 0 \\ 0 & e^{i \frac{2\pi}{2n+1} l} \end{pmatrix}$$

$$\begin{pmatrix} 0 & e^{-i \frac{4\pi}{2n+1} l} \\ e^{i \frac{4\pi}{2n+1} l} & 0 \end{pmatrix}$$

In many situations, we want to real basis (chemists like) this set

$$|\psi_x^{E_1}\rangle = \frac{1}{\sqrt{2}} (|\psi_+^{E_1}\rangle + |\psi_-^{E_1}\rangle) = \frac{1}{\sqrt{2}} \sum_{j=1}^{2n+1} \cos \frac{2\pi}{2n+1} (j-1) |j\rangle \leftarrow P_x$$

$$|\psi_y^{E_1}\rangle = \frac{i}{\sqrt{2}} (|\psi_+^{E_1}\rangle - |\psi_-^{E_1}\rangle) = \frac{i}{\sqrt{2}} \sum_{j=1}^{2n+1} \sin \frac{2\pi}{2n+1} (j-1) |j\rangle \leftarrow P_y$$

Then $(|\psi_x^{E_1}\rangle, |\psi_y^{E_1}\rangle) = (|\psi_+^{E_1}\rangle, |\psi_-^{E_1}\rangle) \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} \leftarrow \text{define as } U$

⇒ The representation matrix

$$\begin{pmatrix} \langle \psi_x^x | \\ \langle \psi_y^x | \end{pmatrix} O (|\psi_+^x\rangle, |\psi_-^x\rangle) = U \begin{pmatrix} \langle \psi_+^E | \\ \langle \psi_-^E | \end{pmatrix} O (|\psi_+^{E_1}\rangle, |\psi_-^{E_1}\rangle) U$$

Representation matrix in the previous basis

⇒ The $C_{2n+1}^l \rightarrow$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} e^{-i\frac{2\pi}{2n+1}l} & 0 \\ 0 & e^{i\frac{2\pi}{2n+1}l} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \cos \frac{2\pi}{2n+1} l & \sin \frac{2\pi}{2n+1} l \\ -\sin \frac{2\pi}{2n+1} l & \cos \frac{2\pi}{2n+1} l \end{pmatrix}$$

$$C_2: \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & e^{-i\frac{4\pi}{2n+1}l} \\ e^{i\frac{4\pi}{2n+1}l} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \cos \frac{4\pi}{2n+1} l & -\sin \frac{4\pi}{2n+1} l \\ -\sin \frac{4\pi}{2n+1} l & -\cos \frac{4\pi}{2n+1} l \end{pmatrix}$$

clearly, this is a real representation.

For other representations E_m : under the angular momentum eigen-basis $\pm m$

$$|\psi_{\pm}^{E_m}\rangle = \frac{1}{\sqrt{2n+1}} \sum_{j=1}^{2n+1} e^{-i \frac{2\pi}{2n+1} m(j-1)} |j\rangle$$

The cyclic rotation C_{2n+1}^l :
$$\begin{bmatrix} e^{-i \frac{2\pi}{2n+1} ml} & 0 \\ 0 & e^{i \frac{2\pi}{2n+1} ml} \end{bmatrix}$$

and the C_2 rotation around

the axis at the angle $\frac{2\pi}{2n+1} l$
$$C_2^l : \begin{bmatrix} 0 & e^{-i \frac{4\pi}{2n+1} ml} \\ e^{i \frac{4\pi}{2n+1} ml} & 0 \end{bmatrix}$$

Again this Rep is actually real: under the basis of

$$(|\psi_{\cos}^{E_m}\rangle, |\psi_{\sin}^{E_m}\rangle) = (|\psi_+^{E_m}\rangle, |\psi_-^{E_m}\rangle) \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix}$$

we have : C_{2n+1}^l :
$$\begin{bmatrix} \cos \frac{2\pi}{2n+1} ml & \sin \frac{2\pi}{2n+1} ml \\ -\sin \frac{2\pi}{2n+1} ml & \cos \frac{2\pi}{2n+1} ml \end{bmatrix}$$

the l -th C_2 :
$$\begin{bmatrix} \cos \frac{4\pi}{2n+1} ml & -\sin \frac{4\pi}{2n+1} ml \\ -\sin \frac{4\pi}{2n+1} ml & -\cos \frac{4\pi}{2n+1} ml \end{bmatrix}$$

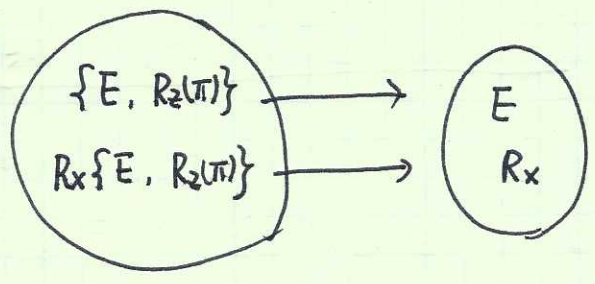
In general

	E	$2C_{2n+1}^1$	$2C_{2n+1}^2$...	$2C_{2n+1}^l$...	$2C_{2n+1}^n$	$(2n+1)C_2$
A_1	1	1	1	1	1	...	1	1
A_2	1	1	1	1	1	...	1	-1
E_1	2	$2\cos \frac{\pi}{2n+1}$	$2\cos \frac{2\pi}{2n+1}$...	$2\cos \frac{2\pi l}{2n+1}$...	$2\cos \frac{2\pi n}{2n+1}$	0
...								
E_m	2	$2\cos \frac{m\pi}{2n+1}$	$2\cos \frac{2m\pi}{2n+1}$...	$2\cos \frac{ml \cdot 2\pi}{2n+1}$...	$2\cos \frac{2\pi mn}{2n+1}$	0
...								
E_n	2	$2\cos \frac{n\pi}{2n+1}$	$2\cos \frac{2n\pi}{2n+1}$...	$2\cos \frac{n l \cdot 2\pi}{2n+1}$...	$2\cos \frac{n^2 \cdot 2\pi}{2n+1}$	0

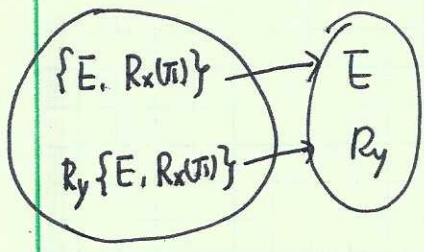
The analysis for the non-abelian group D_{2n} can be done similarly. which will be left for homework.

Below let me show the Rep of D_2 group. = $\{E, R_x(\pi), R_y(\pi), R_z(\pi)\}$. It's an Abelian group, hence it has 4-representations. It has 3 normal subgroups $\{E, R_z(\pi)\}$, $\{E, R_x(\pi)\}$, and $\{E, R_y(\pi)\}$. For each of them, their quotient group is simply Z_2 , and can generate a representations for D_2 .

For example:

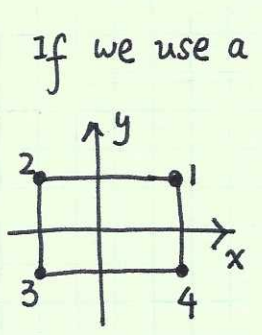


This gives rise to two representations mapping $\{E, R_z(\pi)\}$ to 1. They are called A_1 and A_2 .
 \nearrow if $R_x \rightarrow 1$ \nwarrow if $R_x \rightarrow -1$.



This will generate another new 1d Representation we call it as B_1 . If we use $\{E, R_y(\pi)\}$ as a normal subgroup, we get another one. These two are called B_1, B_2 .

	E	$R_z(\pi)$	$R_x(\pi)$	$R_y(\pi)$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1



If we use a rectangular geometry

$$\begin{aligned} |\psi_{A_1}\rangle &= \frac{1}{2}(|1\rangle + |2\rangle + |3\rangle + |4\rangle) \\ |\psi_{A_2}\rangle &= \frac{1}{2}(|1\rangle - |2\rangle + |3\rangle - |4\rangle) \\ |\psi_{B_1}\rangle &= \frac{1}{2}(|1\rangle - |2\rangle - |3\rangle + |4\rangle) \\ |\psi_{B_2}\rangle &= \frac{1}{2}(|1\rangle + |2\rangle - |3\rangle - |4\rangle) \end{aligned}$$

These 4-1D representations remain for other D_{2n} groups.

If n is even, we have integer angular momentum

$$j_z = 0, \pm 1, \dots, \pm\left(\frac{n}{2}-1\right), \frac{n}{2}$$

$$\pm\frac{1}{2}, \pm\frac{3}{2}, \dots, \pm\frac{n-1}{2}$$

$$\chi_{j_z}(R^l) = e^{-ij_z \cdot l \cdot \theta} \quad \text{with } \theta = \frac{2\pi}{n}$$

Again only $j_z = 0, \frac{n}{2}$, the representations are real, otherwise they are complex. $\rightarrow \chi_{j_z = \frac{n}{2}}(R^l) = (-1)^l$.

Double group of dihedral groups.

Let's begin with D_2 , whose double group is the Quaternion group $Q \cong D_2^D$.

The E and \bar{E} are two classes, since they commute with all other elements. $R_x(\pi)$ and $\bar{R}_x(\pi) = R_x(3\pi)$ are also in the same class, since

$$\bar{R}_x(\pi) = R_x(-\pi) = R_{-\hat{x}}(\pi) \text{ and } \hat{x} \text{ is a bilateral axis. So do}$$

$R_y(\pi)$ and $\bar{R}_y(\pi)$, $R_z(\pi)$ and $\bar{R}_z(\pi)$. Hence there are 5 classes. Q or

D_2^D has a normal subgroup $\{E, \bar{E}\}$, thus the quotient group is D_2 ,

hence all the previous four 1D representations remain a representation of

D_2 . According to $\underbrace{1^2 + 1^2 + 1^2 + 1^2}_{D_2} + \underbrace{2^2}_{\uparrow \text{ spinor Rep.}} = 8$, we have a new spin-1/2 representation.

⊗ Now we consider double group — discrete subgroup of $SU(2)$

For $SU(2)$ group, rotation 360° is different from 0° . We denote this element as \bar{E} . \bar{E} also commutes with all other elements, The double group has twice number of elements compared with the original group.

Double group of the cyclic group — Z_n

$$\{R_z(0), R_z(\frac{2\pi}{N}), \dots, R_z(2\pi), R_z((1+\frac{1}{N})2\pi) \dots R_z[(2-\frac{1}{N})2\pi]\}$$

$$\begin{matrix} \uparrow & & \uparrow & & \uparrow \\ E & & E & & \bar{E} R_z(\frac{2\pi}{N}) \end{matrix}$$

This remains an Abelian group, isomorphic to Z_{2n} , hence, it's not essentially a new group. Nevertheless, the physically interpretation of Reps are different.

- If n is odd, we have integer angular momentum Rep with $j_z = 0, \pm 1, \dots, \pm (n-1)/2$. — These are representations of Z_n .

Now j_z can also take half integer angular momentum

$$j_z = \pm 1/2, \pm 3/2, \dots, \pm \frac{n-2}{2}, \frac{n}{2} \leftarrow \frac{n}{2} \equiv -\frac{n}{2} \pmod{n}$$

j_z	E	R	R ²	...	R ⁿ⁻¹	\bar{E}	$\bar{E}R$...	$\bar{E}R^{n-1}$
0	1	1	1	...	1	1	1	...	1
$\pm m$	1	$e^{\pm im\theta}$	$e^{\pm 2im\theta}$...	$e^{\pm i(n-1)m\theta}$	1	$e^{\pm im\theta}$...	$e^{\pm i(n-1)m\theta}$
$\pm 1/2$	1	$e^{\pm i\frac{\theta}{2}}$	$e^{\pm i\frac{(n-1)\theta}{2}}$	-1	$-e^{\pm i\frac{\theta}{2}}$...	$-e^{\pm i\frac{(n-1)\theta}{2}}$
\dots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
$n/2$	1	-1	1	...	1	-1	1	...	-1

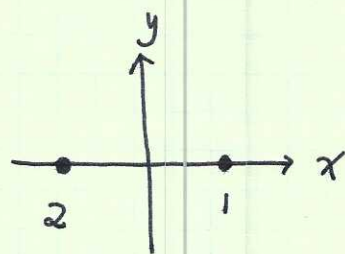
which are the same Reps.

$$\theta = \frac{2\pi}{n}$$

↳ cf. the character table of Z_{2n} .

Then we have

	E	\bar{E}	$R_z \bar{R}_z$	$R_x \bar{R}_x$	$R_y \bar{R}_y$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
$E_{1/2}$	2	-2	0	0	0



$|1\uparrow\rangle, |1\downarrow\rangle$
 $|2\uparrow\rangle, |2\downarrow\rangle$

Let's consider just 2 points, but now with spin. They form a 4-d representation. Under $R_z, \bar{R}_z, R_x, \bar{R}_x, R_y, \bar{R}_y$, there're no diagonal terms, their characters are simply 0. Then $\chi = (4, 4, 0, 0, 0)$, hence it contains two $E_{1/2}$, i.e. $E_{1/2} \oplus E_{1/2}$.

We can choose $|\psi_{E_{1/2}\uparrow}\rangle = \frac{1}{\sqrt{2}} [|1\uparrow\rangle + |2\uparrow\rangle]$, $|\psi_{E_{1/2}\downarrow}\rangle = \frac{1}{\sqrt{2}} [|1\downarrow\rangle + |2\downarrow\rangle]$

note $e^{-i\frac{\sigma_z}{2}\pi} = \begin{pmatrix} -i & \\ & i \end{pmatrix}$, $e^{-i\frac{\sigma_x}{2}\pi} = -i\sigma_x = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$, $e^{-i\frac{\sigma_y}{2}\pi} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

Hence: $E(\bar{E}) : \begin{pmatrix} \pm 1 & \\ & \pm 1 \end{pmatrix}$, $R_z(\bar{R}_z) : \begin{pmatrix} \mp i & \\ & \pm i \end{pmatrix}$,

$R_x(\bar{R}_x) : \begin{pmatrix} 0 & \mp i \\ \mp i & 0 \end{pmatrix}$ $R_y(\bar{R}_y) : \begin{pmatrix} 0 & \pm 1 \\ \mp 1 & 0 \end{pmatrix}$

$\frac{1}{|G|} \sum_g \chi(g^2) = \frac{1}{8} (\chi(E) + \chi(E) + \chi(\bar{E}) + \chi(\bar{E}) + \dots) = \frac{1}{8} (-4 \times 2) = -1$

Hence it's pseudo-real!

no basis for a purely real representation

If we use $|\psi'_\uparrow\rangle = \frac{1}{\sqrt{2}} [|1\uparrow\rangle - |2\uparrow\rangle]$, $|\psi'_\downarrow\rangle = \frac{1}{\sqrt{2}} [|1\downarrow\rangle - |2\downarrow\rangle]$

then please check that, we will have

$$E(\bar{E}) = \begin{pmatrix} \pm 1 & \\ & \pm 1 \end{pmatrix}, \quad R_z(R_{\bar{z}}) = \begin{pmatrix} \pm i & 0 \\ 0 & \mp i \end{pmatrix}, \quad R_x(R_{\bar{x}}) = \begin{pmatrix} 0 & \mp i \\ \mp i & 0 \end{pmatrix}$$

$$R_y(\bar{R}_y) = \begin{pmatrix} 0 & \mp 1 \\ \mp 1 & 0 \end{pmatrix}.$$

These two representations are equivalent. Can you find the matrix to connect them?