33-780 Nuclear and Particle Physics II
Note 5 Tensor Method in $SU(n)$

October 14, 2012

Contents

Physical Application of Finite Group

1 Crystal Symmetry

A crystalline solid is a regular array which is invariant under translation of the form,

$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

In addition, there are also rotations which can be carried in a unit cell of the crystal.

Space group–the complete operations of a crystal, including translation and rotations

Point group–only rotations

It turns out there are only 32 space groups which are consistent with translational invariant

1.1 Point group

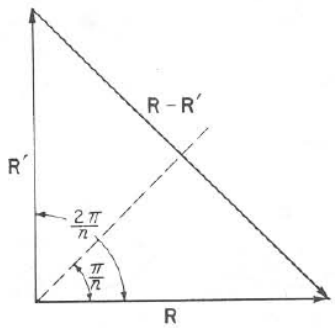
1. C_n –point group with one n-fold symmetry axis only

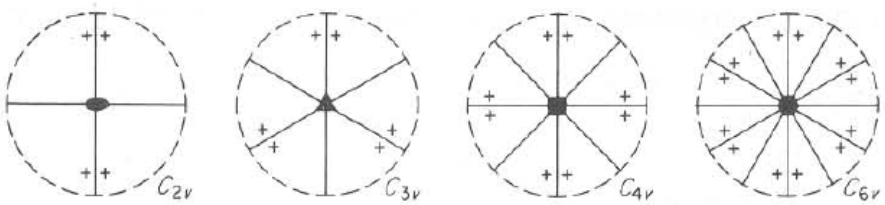
   n can only be $2, 3, 4, 6$ in order to be consistent with translational invariant

   Write the translation in plane perpendicular to the rotation axis the form,

   $$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

   Let $\vec{R}$ be the one with shortest length. Rotate this by $\dfrac{2\pi}{n}$ to get another translation $\vec{R}'$ which will have the same length as $\vec{R}$. Consider the combination $\vec{R} - \vec{R}'$.





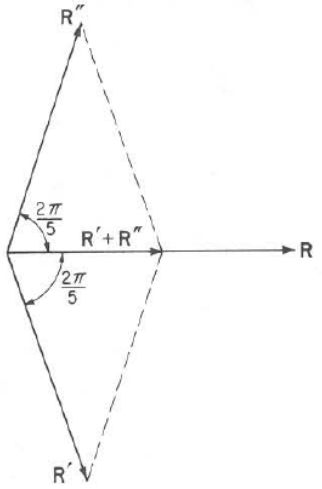
From the figure it is seen that

$$\left|\vec{R} - \vec{R}'\right| = 2R\sin\frac{2\pi}{n}$$

Since $\vec{R}$ is the shortest length we require

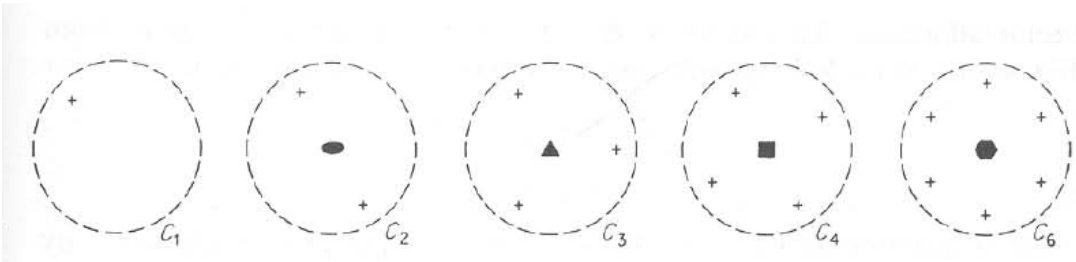
$$2R\sin\frac{2\pi}{n} \leq R$$

This implies that $n \leq 6$.



For the case $n = 5$, we can show that $\left|\vec{R} + \vec{R}'\right| \geq R$ and is ruled out.

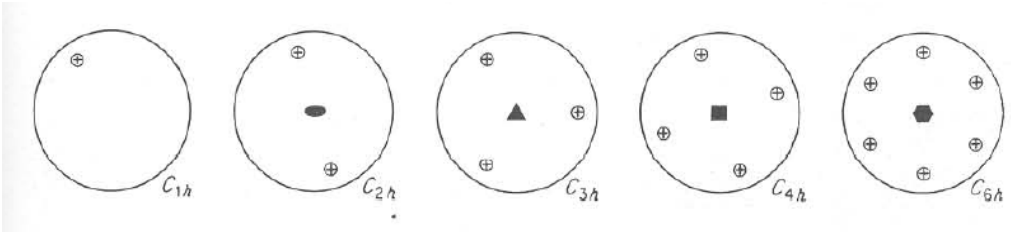
Possible C_n symmetries are given below;



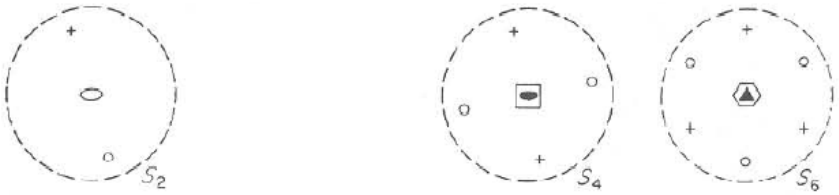
These are all cyclic Abelian groups.

2. $C_{nv}-$ In addition to C_n axis there is a vertical reflection plane σ_v , reflection in a plane passing through the axis of highest symmetry. Solid lines indicate the vertical reflection planes.

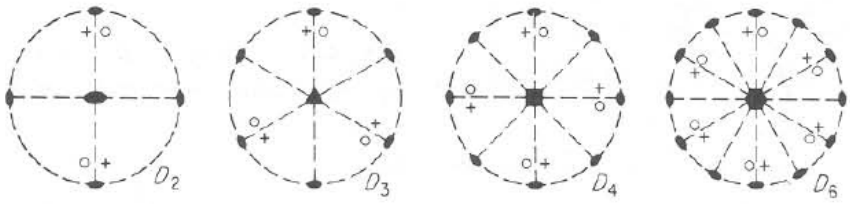
3. $C_{nh}-$There is a horizontal reflection plane $\perp$ to C_n, the axis of highest symmetry.



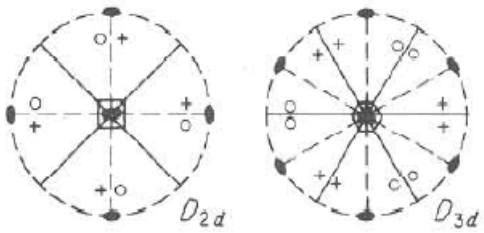
4. S_n- These groups have improper rotation through $\dfrac{2\pi}{n}$.
   Improper rotation–rotation followed by reflection in the plane $\perp$ to axis of rotation
   If n is odd these groups are identical to C_{nh}



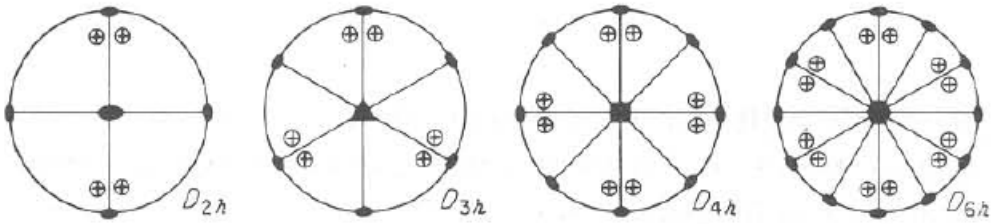
5. D_n- These groups have n twofold axes $\perp$ to principal C_n axis



6. $D_{nd}-$ In D_n there are additional diagonal reflection planes σ_d, bisecting the angles between 2-fold axies $\perp$ to principal axis.



7. $D_{nh}-$ There are additional horizontal reflection plane σ_h



8. $T-$ Symmetry of tetrahedron. It has 12 proper rotations, 3 C_2, around X, Y, Z axes and 8 C_3 along body diagonals.

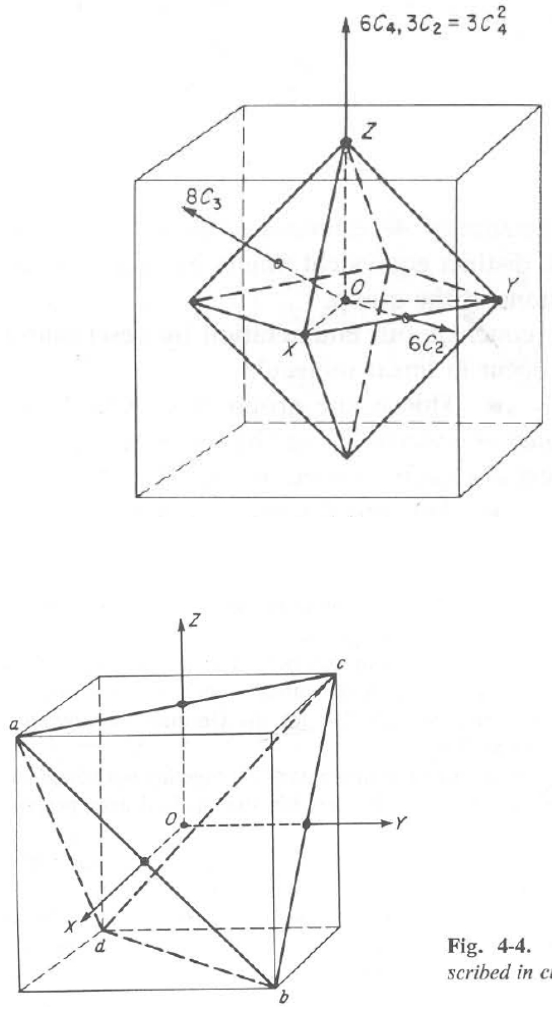
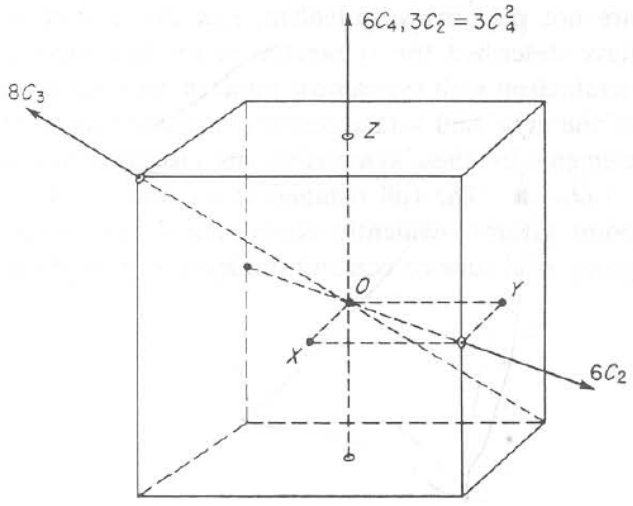


Fig. 4-4. *Tetrahedron inscribed in cube.*

9. T_d- This group contains reflections in addition to those in T.



10. $O-$ *Octahedral group*$-$ proper rotations which take a cube or an octahedron into itself. This group has 8 C_3 along body diagonals, 3 C_2, around X, Y, Z axes, and 6 C_4, around X, Y, Z axes

11. $O_h = O \times i$ This group includes improper rotations and reflections

1.2 Elementary rep of rotation group

One simple application of group theory is to study the effect of crystal fields on the atom if the field is weak enough. For this we need to study the rotational properties of a free atom. We study the representation of full rotation group in details in next chapter. Here we will just borrow some simple results for our purpose. As we learn from Quantum Mechanics that irreps are labelled by orbital angular momentm l which takes integer values, $l = 0, 1, 2, 3, \cdots$ and we can take spherical harmonics as the basis functions,

$$Y_l^m(\theta, \phi) \sim P_l^m(\theta) e^{im\phi}, \qquad m = -l, \cdots, l$$

where $P_l^m(\theta)'s$ are the associated Legendre functions. Under the rotation R we have,

$$P_R Y_l^m = \sum_m \Gamma^{(l)}(R)_{m'm} Y_l^{m'}$$

We need to know the characters of these representations in order to study how they split up under the crystal fields. We will use the property that rotations with same angle are all in the same class and choos the simple case of rotation of angle α around $z - axis$. In this case we get

$$P_\alpha Y_l^m(\theta, \phi) = Y_l^m(\theta, \phi - \alpha) = e^{-im\alpha} Y_l^m(\theta, \phi)$$

The character is then

$$\chi^{(l)}(\alpha) = \sum_{m=-l}^{l} e^{-im\alpha} = \frac{\sin\left(l + \frac{1}{2}\right)\alpha}{\sin\frac{\alpha}{2}}$$

We will use this formula to study the splitting of enegy levels.

1.3 Crytal-field splitting of atomic levels

If we describe the crytal field by a potential, then this potential should be invariant under the symmetry group of the crystal. We will illustrate the splitting of atomic levels reduces by an example. The character table of octahedron group is given below,

		E	$8C_3$	$3C_2$	$6C_2$	$6C_4$
Γ_1	A_1	1	1	1	1	1
Γ_2	A_2	1	1	1	-1	-1
Γ_3	E	2	-1	2	0	0
Γ_4	T_1	3	0	-1	-1	1
Γ_5	T_2	3	0	-1	1	-1

For the atomic levels we use the formula given above with the results,

$$\chi^{(l)}(C_2) = \chi(\pi) = (-)^l$$

$$\chi^{(l)}(C_3) = \chi\left(\frac{2\pi}{3}\right) = \begin{cases} 1 & l = 0, 3, \cdots \\ 0 & l = 1, 4, \cdots \\ -1 & l = 2, 5, \cdots \end{cases}$$

$$\chi^{(l)}(C_4) = \chi\left(\frac{\pi}{2}\right) = \begin{cases} 1 & l = 0, 1, 4, 5 \cdots \\ -1 & l = 2, 3, 6, 7, \cdots \end{cases}$$

With respect to O group we get

O	E	$8C_3$	$3C_2$	$6C_2$	$6C_4$
D_0	1	1	1	1	1
D_1	3	0	-1	-1	1
D_2	5	-1	1	1	-1
D_3	7	1	-1	-1	-1

where we denote $l = n$ representation by D_n. Using the formula for computing the coefficients of reduction of representation, we get

$$D_0 = A_1, \qquad D_1 = T_1, \qquad D_2 = E + T_2, \qquad D_3 = A_2 + T_1 + T_2$$

This gives the splitting of the atomic levels. For example, 5 $l = 2$ levels split into a doublet E, and a triplet T_2.

Additional splitting in field of lower symmetry

In actual crystals there are some small departure from cubic symmetry O. Consider the example the the cubic symmetry O is reduced to D_3. We can study the further splitting again using character table

D_3

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

O

A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
T_1	3	0	-1
T_2	3	0	1

From this we see that $T_1 \longrightarrow E + A_2,\ \ T_2 \longrightarrow E + A_1$. This means that triplet level T_1 will split into a doublet E and a singlet A_2.