Angular momentum in finite point groups

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Contents

1 Introduction

The topic of this seminar are the symmetries of the finite box in three dimensional space. The main goal is to find what sort of fields with correct momenta transform as irreducible representations under the relevant symmetry groups. In order to do this, seminar will be separated in 5 sections, where in Section 2 types of composite fields, that describe the particles in the box will be introduced. We will note, that to have a proper theory these fields need to satisfy some conditions; these conditions however will then have large consequences. In Section 3 the relevant groups $O(3)$, O_h and C_{4v} will be introduced and their properties presented. Section 4 describes a general procedure to obtain good fields, that can be used in lattice simulations. In Section 5 an example where the scattering particles have zero total momentum will presented and in Section 6 an example with smaller symmetry will be obtained by reducing the example from Section 5.

2 Composite fields

Although lattice QCD simulations are done both on meson scattering and barion scattering [also plenty of other stuff], this seminar concentrates on meson scattering. However the procedure is general enough, so that it can be extended to barion barion and meson barion scattering.

A meson is composite field composed of two elementary quark fields:

$$M(\vec{p}) = \int d^3\vec{x} e^{i\vec{p}\vec{x}} \bar{q}(\vec{x}) \Gamma q(\vec{x}), \tag{1}$$

where $q(\vec{x})$ and $\bar{q}(\vec{x})$ are two quark fields at a given point $\vec{x}$ in space, $\vec{p}$ is the momentum to which the composite fields are projected to. This means that $\vec{p}$ is the momentum of the meson M. Γ is a product of Dirac matrices, chosen in such a way, that the field has quantum numbers of the meson we want. For instance if the meson is a pion, then it is a pseudoscalar particle, which means that it does not change under rotation, however gets a minus sign under parity transformations. Then $\Gamma = \gamma_5$. Therefore the Γ structure defines how the meson field will act.[1] A vector meson [e.g. ρ] will then be a three component field, each component corresponding to a given polarization of the particle.

Some examples of the possible fields can be written down:

$$f_1 = M(\vec{p}),\ \Gamma \text{ is scalar or pseudoscalar;} \tag{2}$$
$$f_{2i} = M_i(\vec{p}),\ \Gamma \text{ is vector or axial vector;} \tag{3}$$
$$f_3 = M(\vec{p}_1)M^{'}(\vec{p}_2); \tag{4}$$
$$f_4 = M_i(\vec{p}_1)M_i^{'}(\vec{p}_2); \tag{5}$$
$$f_{5i} = M_i(\vec{p}_1)M^{'}(\vec{p}_2); \tag{6}$$

f_1 and f_2 correspond to single meson fields, while f_3, f_4 and f_5 are double meson fields [physically these describe scattering channels, while the previous describe "all" possible states]. Field f_3 will be of main interest in this seminar.

At this point the physical system that is of concern to this seminar will be described. This is a finite box with periodic boundary conditions; meaning that the momenta particles can have are limited to those momenta, that satisfy the boundary conditions. At this point the momenta are not limited to some specific values, only the fact, that they are no longer a continuous variable [they are countably infinite actually]. This means, that the integral in Equation 1 now becomes a sum over all allowed momenta denoted by $\vec{d}$:

$$M(\vec{p}) = \int d\vec{x} e^{i\vec{p}\vec{x}} \bar{q}(\vec{x}) \Gamma q(\vec{x}), \vec{p} \text{ satisfies periodic b.c.} \tag{7}$$

So in order to have a proper theory, the momentum $\vec{p}$ in Equation 7 can only have values, that satisfy periodic boundary conditions. This is the condition of the system and from this it follows, that field combinations with specific momenta $\vec{p}$ need to be found. Before doing this, relevant groups will be introduced in the following section.

3 Relevant groups

The relevant groups needed in this seminar are the $O(3)$ continuous group, its subgroup the octahedral point group O_h and the ditetragonal pyramidal point group C_4v. Their geometric representation, symmetry transformations and group character tables will be listed in the following subsections.

[1]For the purpose of this seminar this holds, however when charge parity is considered, then gauge operators in a resulting meson field would also affect its quantum number.

3.1 $O(3)$

The $O(3)$ group is the group of 3×3 real matrices with determinant $\det T(O(3)) = \pm 1$. Sometimes it is also written as $O(3, \mathbb{R})$, where $\mathbb{R}$ denotes that it is over the real numbers. It is worth noting, that angular momentum, only has $SO(3)$ symmetry, which means that matrices with $\det T(O(3)) = -1$ are not included. Therefore space inversion, or also known as parity, is not in the $SO(3)$ group, however it is still a symmetry of the box and of the meson fields in it. It is this reason, why the $O(3)$ group is considered. However the way it will be considered is by writing it as the $SO(3)$ for the elements that have $\det T(O(3)) = 1$ combined with parity for the rest of the elements; $O(3) = SO(3) \times Z_2$

Geometric interpretation of the $O(3)$ continuous group is presented in Figure 3. It is a unit sphere, which represents, how a unit vector $\vec{r}$ can be transformed under the transformations that form the $O(3)$ symmetry group.

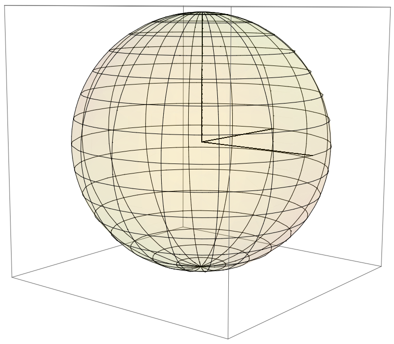

Figure 1: Geometric interpretation of $O(3)$ symmetry; unit sphere.

The transformations that form the $O(3)$ group are the transformations of the $SO(3)$ group combined with inversion. A general element of $O(3)$ is then the product of identity or inversion and rotation for angle α around some axis $\vec{d}$.:

$$\begin{aligned}
&\text{case of } \det T(O(3)) = 1: \\
&R(\alpha, \vec{d}) = e^{-i\alpha \vec{d}.\vec{L}} \qquad (8)\\
&\text{case of } \det T(O(3)) = -1: \\
&R^{'}(\alpha, \vec{d}) = -I\ e^{-i\alpha \vec{d}.\vec{L}}, \qquad (9)
\end{aligned}$$

where L_i are generators of the continuous group $SO(3)$[in real space]:

$$L_x = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad L_y = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad L_z = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \qquad (10)$$

These are the rotation matrices in coordinate space, however much more interesting is what happens in wave function space. The states with $O(3)$ symmetry can be characterized with 3 numbers: l which denotes the representation [it also describes the angular momentum value], m which is the projection of l on the z axis, and P which denotes parity. In case when $P = +1$ this is the $SO(3)$ subgroup with positive parity states and when $P = -1$ this is the $SO(3)$ group with negative parity states. This is then the $O(3)$ group, which could also be written as the direct product $SO(3) \times Z_2$, where Z_2 stands for parity symmetry.

As matrices R and R' describe how the coordinate vectors rotate, a wave function basis of spherical harmonics $Y_{lm}(\theta, \phi)$, which span the space of functions on a unit sphere is introduced; meaning that any given function on a unit sphere can be written as a linear combination of spherical harmonics. Rotation matrices on these states can be defined as:

$$D^l_{m,m'}(\alpha, \vec{d}) = \frac{1}{4\pi} \int d\Omega Y^*_{lm}(\theta, \phi) R^{(')}(\alpha, \vec{d}) Y_{lm'}(\theta, \phi), \tag{11}$$

and then the rotation of states is written as:

$$Y'_{lm} = \sum_{m'} D^l_{m,m'} Y_{lm'}. \tag{12}$$

The unitary matrices $D^l_{m,m'}$ are also called the Wigner D matrices in the case they only describe rotations. In the case above they describe also reflections over mirror planes and improper rotations.

Characters for the representations l and given transformations are needed. For the case of the $SO(3)$ subrgoup this is straightforward, however for the rest it will be provided.
The characters of transformations of $SO(3)$ will be the same for a given angle of rotation no matter the axis of rotation. A simple way to see this is to consider a rotation through α about vector $\vec{e}_u$, $R_{\vec{e}_u}(\alpha)$. To get a rotation through α about vector $\vec{e}_v$, a rotation through an angle δ about a vector $\vec{e}_n$, $R_{\vec{e}_n}(\delta)$ is needed. Then the rotation through α about $\vec{e}_v$ is:

$$R_{\vec{e}_v}(\alpha) = R_{\vec{e}_n}(\delta) R_{\vec{e}_u}(\alpha) R^{-1}_{\vec{e}_n}(\delta). \tag{13}$$

Note that the matrices R can be in any given representation; specifically they are interesting in the space of spherical harmonics. The character of a representation for a given α is from this obviously independent of the vector about which the rotation is, and only depends on the angle the rotation rotates for. This is due to the fact, that the character is defined as the trace of a matrix representation; the trace has a cyclicty property, from which it follows:

$$Tr[A] = Tr[RAR^{-1}] = Tr[R^{-1}RA] \tag{14}$$

Now the characters for the $SO(3)$ can be determined simply by considering rotations for a given angle about the z axis:

$$R_{\vec{z}}(\alpha) Y_{lm}(\theta, \phi) = Y_{lm}(\theta, \phi + \alpha) = \sum_{m'} D^l_{m,m'}(\vec{z}, \alpha) Y_{lm}(\theta, \phi), \text{ where} \tag{15}$$

$$Y_{lm}(\theta, \phi + \alpha) = e^{im\alpha} Y_{lm}(\theta, \phi) \tag{16}$$

$$\chi^l(\alpha, proper) = \sum_m D^l_{mm}(\vec{z}, alpha) = \sum_{m=-l}^{l} e^{im\alpha} \tag{17}$$

$$= \frac{-e^{i\alpha l} + e^{i\alpha l} e^{i\alpha}}{-1 + e^{i\alpha}} = \frac{\sin{(l + 1/2)\alpha}}{\sin{\alpha/2}}. \tag{18}$$

In short for the $SO(3)$ subgroup of the $O(3)$ group the characters of the transformations will be independent on the axis of rotation, however will be different for different angles of rotation. The other part of the $O(3)$ group consists of improper rotations, meaning a rotation and an inversion. The characters of such transformations will then have a -1 prefactor depending on the representation:

$$\chi^l(\alpha, improper) = (-1)^l \frac{\sin{(l + 1/2)(\alpha + \pi)}}{\sin{(\alpha + \pi)/2}}. \tag{19}$$

Using the above relations, characters for any given representation of the $O(3)$ symmetry group can be calculated.

3.2 O_h

The O_h group is the octahedral point group with added inversion [1]. It is the symmetry of a (empty) box. Sometimes the octahedral group can be written as $O(3, \mathbb{Z})$, where $\mathbb{Z}$ denotes, that the group is over whole numbers; the representations will up to normalization be constructed from whole numbers only. It is a finite subgroup of $O(3, \mathbb{R})$, meaning that it also includes parity.

Geometric interpretation of the octahedral group is a cube. The transformations that form the

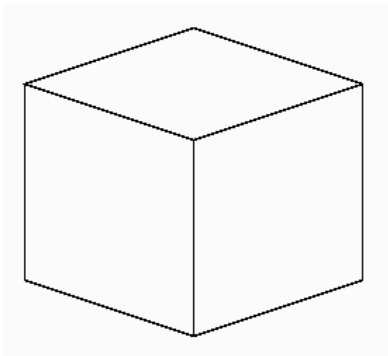

Figure 2: Geometric interpretation of O_h symmetry; the cube

octahedral group leave the cube invariant under them.

The octahedral group consists of the following transformations:

- identity E [does nothing],
- 8 threefold rotations [a rotation for $2\pi/3$ about some axis; for example the (1,1,1) axis],
- 3 fourfold rotations repeated twice [rotation for $\pi/2$ twice; for example the (0,0,1) axis],
- 6 twofold rotations [rotations for π; for example the (0,0,1) axis],
- 6 fourfold rotations [rotations for $\pi/2$; for example the (0,0,1) axis],
- inversion [$\vec{r} \to -\vec{r}$],
- 6 fourfold improper rotations [a fourfold rotation followed by reflection through the principal axis of the rotation],
- 8 sixfold improper rotations [a sixfold rotation followed by a reflection through the principal axis of rotation; for example the (1,1,1) axis],
- 3 reflections through a horizontal plane,
- 6 reflections through a diagonal plane.

From above we can see, that O_h has 48 elements divided into 10 classes. It has 10 irreducible representations, that can be divided into 5 irreducible representations for each parity. They are denoted as:

$A_1^{\pm}$, $A_2^{\pm}$, $E^{\pm}$, $T_1^{\pm}$, $T_2^{\pm}$ and are 1, 1, 2, 3, 3 dimensional respectively.

We will again be interested in the implications of these on the wave function basis, however they are straight forward to workout from above definitions.

The characters of these transformations in the 10 irreducible representations are given in the character table [2], Table 1.

	E	$8\ C_3$	$6\ C_2$	$6\ C_4$	$3\ C_4^2$	I	$6\ S_4$	$8\ S_6$	$3\ \sigma_h$	$6\ \sigma_d$
A_1^+	1	1	1	1	1	1	1	1	1	1
A_2^+	1	1	-1	-1	1	1	-1	1	1	-1
E^+	2	-1	0	0	2	2	0	-1	2	0
T_1^+	3	0	-1	1	-1	3	1	0	-1	-1
T_2^+	3	0	1	-1	-1	3	-1	0	-1	1
A_1^-	1	1	1	1	1	-1	-1	-1	-1	-1
A_2^-	1	1	-1	-1	1	-1	1	-1	-1	1
E^-	2	-1	0	0	2	-2	0	1	-2	0
T_1^-	3	0	-1	1	-1	-3	-1	0	1	1
T_2^-	3	0	1	-1	-1	-3	1	0	1	-1

Table 1: O_h character table.

3.3 C_{4v}

The ditetragonal pyramidal point group is the point group, obtained by adding reflection symmetry to the point group C_4. The latter is a small and simple group. It has one principal axis and is abelian. However C_{4v} also has reflection symmetry, which renders it nonabelian. The C_{4v} is the symmetry group of transformations that leave the the block element unchanged, however not quite; this block is such, that the upper half is painted gray and the lower half is painted white. This object then has the C_{4v} symmetry. C_{4v} is both a subgroup of $O(3)$ and O_h.

Geometric interpretation is a block, that has different coloring in the upper half than in the lower half.

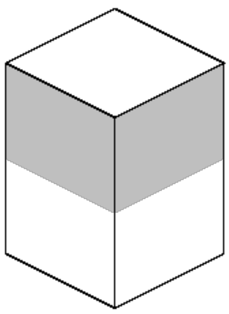

Figure 3: Geometric interpretation of C_{4v} symmetry; colored block.

The ditetragonal pyramidal group consits of the following transformations:

- identity [does nothing]

- 2 fourfold rotations [rotation for $\pi/2$; for example around the (0,0,1) axis]
- 1 twofold rotation [rotation for π; for example around the (0,0,1) axis]
- 2 vertical reflections [reflection through the plane defined by a vector; for example (1,0,0) vector]
- 2 diagonal reflections [for example (1,1,0) vector]

From above it can be seen, that the C_{4v} point group has 8 elements that are divided into 5 classes, It has 5 irreducible representations, however in contrast to O_h, where they were labeled with respect to parity, the C_{4v} point group no longer has inversion symmetry; this is a consequence of coloring. The irreducible representations are $A_1,\ A_2,\ B_1,\ B_2,\ E$, that are 1, 1, 1, 1 and 2 dimensional respectively.

The characters of these transformations in the 5 irreducible representations are given in the character table, Table 2:

	E	$2\ C_4$	C_2	$2\ \sigma_v$	$2\ \sigma_d$
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	2	0	-2	0	0

Table 2: C_{4v} character table

4 General procedure

A general procedure to obtain physically relevant fields which will transform irreducibly with respect to the symmetry of the finite box they are in. This consists of first obtaining the decomposition of the full symmetry to the symmetry of the box. Some information on physics can already be obtained from here. However for full significance a specific formula of projection operators can be used to obtain the basis vectors or actually the correct linear combinations of the relevant fields, that then allows proper determination of states.

To see how the the full symmetry decomposes under the smaller symmetry, characters for irreducible representations of the full and the smaller symmetry need to be known. For clarity A will be denoted as the full symmetry, while B will be denoted as the small symmetry. The "size" is classified with respect to number of elements in the group, g. The representations, that transform as irreducible under the symmetry A, transform as reducible under the transformations of B. The decomposition of A in B is then defined by [3]:

$$m_{B,i} = \frac{1}{g}\sum_R \chi^A(R)\chi^{B,i}(R), \tag{20}$$

where m_B is the number, that denotes how many times does a irreducible representation of B appear in the given representation of A; specifically the representation of A, that transforms as irreducible under A.

The result of such a decomposition is given as a direct sum of representations. Let Γ^A denote a representation of A and Γ_i^B as the $i-th$ irreducible representation of B. Note that Γ^A can transform as irreducible under the transformations of the group A and as reducible under the transformations of group B. Then the decomposition is:

$$\Gamma^A = m_{B,1}\Gamma_1^B \oplus m_{B,2}\Gamma_2^B \oplus ... \tag{21}$$

The sum goes over all the irreducible representations of group B.

Remember that in $O(3)$, the representation is labeled by l, which is what is physically called angular momentum. From the decomposition of A= $O(3)$ and B= O_h we can determine which angular momenta will be excited with fields, that are in a given irreducible representation of B. Physically this means fields with specific combinations of momenta. This is of crucial importance to be able to determine the physical states.

However to be able to determine the precise field combinations of the fields, that will excite specific angular momenta, projection operators need to be deployed. Projection operators are usually defined as:

$$P_i^B = \frac{s_B}{g}\sum_R T_{ii}^B(R)T^A(R), \tag{22}$$

where s_B is dimensionality of the irreducible representation B, R are the elements of the group B, $T_{ii}^B(R)$ are diagonal elements of the irreducible representation and $T^A(R)$ are the elements of the group B in some reducible representation.
This projection operator projects the transformations in A, that are reducible in B to some eigenvectors of irreducible representations of B. However this projection operator is not what is most useful, as $T_{ii}^A(R)$ for each i and R are needed. This is less than advantageous, so therefore an alternative projection operator can be defined. It is not formally denoted as a projection operator, however for the duration of this seminar it will be named projection operator. The new projection operator will be a sum over all i. This means, that the projection operator becomes:

$$P^B = \frac{s_B}{g}\sum_R \chi^B(R)T^A(R). \tag{23}$$

The result of this is a matrix, which has some eigenvectors; these are the sums of the eigenvectors of a given irreducible representation B. In order to obtain true eigenvectors, a Gramm-Schmidt procedure is required to obtain an orthonormal basis of a the irreducible representation B. Many times it happens, that this matrix is block diagonal with already orthogonal eigenvectors, which means that the Gramm-Schmidt procedure can be skipped.

With the given projection operator, field combinations that couple only to specific[up to some extent] angular momenta can be created; excited states can therefore be recognized and determined.

5 Decomposition of $O(3)$ in O_h

To determine the decomposition, Equation (20) requires the characters of both groups, the continuous group $O(3)$ and the point group O_h. The characters of the group O_h are explicitly provided in Table 1, while for the $O(3)$ group only a prescription how to obtain them was given. In order to do to the decomposition, the relevant characters need to be obtained. That is the characters of the following transformations under $O(3)$[2]:

[2]The reflections can be expressed as $\sigma = IC_2$, first do a twofold rotation and then do the inverse; or the other way around – they commute.

- identity: $\chi^{l=0}(0) = 1$, $\chi^{l=1}(0) = 3$
- threefold rotation: $\chi^{l=0}(2\pi/3) = 1$, $\chi^{l=1}(2\pi/3) = 0$
- twofold rotation: $\chi^{l=0}(\pi) = 1$, $\chi^{l=1}(\pi) = -1$
- fourfold rotation: $\chi^{l=0}(\pi/2) = 1$, $\chi^{l=1}(\pi/2) = 1$
- twofold rotation: $\chi^{l=0}(\pi) = 1$, $\chi^{l=1}(\pi) = -1$
- inversion: $\chi^{l=0} = 1$, $\chi^{l=1} = -3$
- improper fourfold rotation: $\chi^{l=0} = 1$, $\chi^{l=1} = -1$
- improper sixfold rotation: $\chi^{l=0} = 1$, $\chi^{l=1} = 0$
- horizontal reflection: $\chi^{l=0} = 1$, $\chi^{l=1} = 1$
- diagonal reflection: $\chi^{l=0} = 1$, $\chi^{l=1} = 1$

Higher l are not presented, however could be calculated by given prescription. Thus the decompositions are quite simple:

$$l = 0 \to A_1^+, \tag{24}$$
$$l = 1 \to T_1^-. \tag{25}$$

However a different presentation of this will be more enlightening:

$$A_1^+ \to l = 0, 4, ... \tag{26}$$
$$T_1^- \to l = 1, 3, ... \tag{27}$$

Here it can be seen, that not all plane waves are present in a specific representation [the decomposition provided here is a bit larger for clarity]. Indeed the A_1^+ irreducible representation mixes only $l = 0$ and $l = 4$ waves. The T_1^- mixes $l = 1, 3$ waves.

5.1 Projection operators and final fields

An example of the above decomposition follows. Fields with $O(3)$ symmetry from Section 2 with general momenta, will get limited momenta, such that they no longer have $O(3)$ symmetry. From these a reducible basis will be written and then the use of projection operators demonstrated on a specific representation, to obtain eigenvectors of this specific irreducible representation.

Among the possible fields that present meson meson scattering the following is chosen:

$$\psi = M(\vec{p})M^{'}(-\vec{p}) = f_3. \tag{28}$$

Due to the fact, that there are no boundary conditions on $\vec{p}$, this field has $O(3)$ symmetry. However when this field is put in a finite box with periodic boundary conditions, then $\vec{p}$ is no longer a continuous variable, but a discrete one. It can only have values:

$$\vec{p} = \frac{2\pi}{L}\vec{n}, \quad \vec{n} \in \mathbb{Z}^3. \tag{29}$$

The simplest and smallest momenta $\vec{n}$ can take are:

$$\vec{n}_1 = (1,0,0), \qquad \vec{n}_2 = (-1,0,0), \tag{30}$$
$$\vec{n}_3 = (0,1,0), \qquad \vec{n}_4 = (0,-1,0), \tag{31}$$
$$\vec{n}_5 = (0,0,1), \qquad \vec{n}_6 = (0,0,-1). \tag{32}$$

Then the meson fields are:

$$\psi_1 = M(\vec{n}_1)M(-\vec{n}_1), \tag{33}$$
$$\psi_2 = M(\vec{n}_2)M(-\vec{n}_2), \tag{34}$$
$$\psi_3 = M(\vec{n}_3)M(-\vec{n}_3), \tag{35}$$
$$\psi_4 = M(\vec{n}_4)M(-\vec{n}_4), \tag{36}$$
$$\psi_5 = M(\vec{n}_5)M(-\vec{n}_5), \tag{37}$$
$$\psi_6 = M(\vec{n}_6)M(-\vec{n}_6), \tag{38}$$
$$\tag{39}$$

We will take these to span our space. Obviously in continuous space the plane wave expansion is an infinite series. Even in the case of discrete momenta this somewhat holds, as noted before, now certain representations mix only certain l waves. What is actually most important in lattice simulations, to have as little plane waves in a representation as possible. This happens, if irreducible representations of the finite box are employed.

The fields now have a basis, however it is in a reducible form. In order to get correct combinations, that lead to irreducible representations, the use of projection operators is needed. To obtain projection operators, the transformations of the fields with the above basis is needed. In order to get those, the specific transformations of the O_h group need to be written down. Their actions will be described, however as that is clear, their actions on $\vec{n}_i$ need not be written down explicitly.

- identity - no explanation necessary
- $C_4^+(x,y,z)$: rotation for $\pi/2$ about x,y,z axes respectively
- $C_4^-(x,y,z)$: rotation for $-\pi/2$ about x,y,z axes respectively
- $C_2(x,y,z)$: rotation for π about x,y,z axes respectively
- $C_2((x \pm y))$: rotation for π about $x \pm y$ axes
- $C_2((x \pm z))$: rotation for π about $x \pm z$ axes
- $C_2((y \pm z))$: rotation for π about $y \pm z$ axes
- $C_3^{1,2}(x \pm y + z)$: rotation once or twice for $2\pi/3$ about $x \pm y + z$ axes
- $C_3^{1,2}(-x - y + z)$: rotation once or twice for $2\pi/3$ about $-x - y + z$ axes
- $C_3^{1,2}(x - y - z)$: rotation once or twice for $2\pi/3$ about $x - y - z$ axes
- inversion: $\vec{r} \to -\vec{r}$
- $IC_4^+(x,y,z)$: improper rotation for $\pi/2$ about x,y,z axes respectively
- $IC_4^-(x,y,z)$: improper rotation for $-\pi/2$ about x,y,z axes respectively

- $IC_2(x,y,z)$: reflection through x,y,z defining planes respectively
- $IC_2((x \pm y))$: reflection through plane defined by $x \pm y$ axes
- $IC_2((x \pm z))$: reflection through plane defined by $x \pm z$ axes
- $IC_2((y \pm z))$: reflection through plane defined by $y \pm y$ axes
- $IC_3^{1,2}(x \pm y + z)$: improper rotation once or twice for $2\pi/3$ about $x \pm y + z$ axes
- $IC_3^{1,2}(-x - y + z)$: improper rotation once or twice for $2\pi/3$ about $-x - y + z$ axes
- $IC_3^{1,2}(x - y - z)$: improper rotation once or twice for $2\pi/3$ about $x - y - z$ axes

These transformations have the usual definition in the coordinate vector space, however they also have a representation in the basis of the field vectors defined above: [This is a bit ridiculous to write explicitly; however those needed to calculate the projection operator are...]

$$Id = \begin{pmatrix} 1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1 \end{pmatrix} C_2(x) = \begin{pmatrix} 1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0 \end{pmatrix} C_2(y) = \begin{pmatrix} 0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0 \end{pmatrix},$$

$$C_2(z) = \begin{pmatrix} 0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1 \end{pmatrix} C_4^+(x) = \begin{pmatrix} 1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\\0&0&1&0&0&0\\0&0&0&1&0&0 \end{pmatrix} C_4^+(y) = \begin{pmatrix} 0&0&0&0&1&0\\0&0&0&0&0&1\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&1&0&0&0&0\\1&0&0&0&0&0 \end{pmatrix}$$

$$C_4^+(z) = \begin{pmatrix} 0&0&0&1&0&0\\0&0&1&0&0&0\\1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1 \end{pmatrix} C_4^-(x) = \begin{pmatrix} 1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\\0&0&0&1&0&0\\0&0&1&0&0&0 \end{pmatrix} C_4^-(y) = \begin{pmatrix} 0&0&0&0&0&1\\0&0&0&0&1&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\1&0&0&0&0&0\\0&1&0&0&0&0 \end{pmatrix}$$

$$C_4^-(z) = \begin{pmatrix} 0&0&1&0&0&0\\0&0&0&1&0&0\\0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1 \end{pmatrix} C_2(x{+}y) = \begin{pmatrix} 0&0&1&0&0&0\\0&0&0&1&0&0\\1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0 \end{pmatrix} C_2(x{-}y) = \begin{pmatrix} 0&0&0&1&0&0\\0&0&1&0&0&0\\0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0 \end{pmatrix}$$

$$C_2(x{+}z) = \begin{pmatrix} 0&0&0&0&1&0\\0&0&0&0&0&1\\0&0&0&1&0&0\\0&0&1&0&0&0\\1&0&0&0&0&0\\0&1&0&0&0&0 \end{pmatrix} C_2(x{-}z) = \begin{pmatrix} 0&0&0&0&0&1\\0&0&0&0&1&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&1&0&0&0&0\\1&0&0&0&0&0 \end{pmatrix} C_2(y{+}z) = \begin{pmatrix} 0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\\0&0&1&0&0&0\\0&0&0&1&0&0 \end{pmatrix}$$

$$C_2(y+z) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} Inv = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} IC_2(x) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$IC_2(y) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} IC_2(z) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} IC_4^+(x) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}]$$

$$IC_4^+(y) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} IC_4^+(z) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} IC_4^-(x) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$$IC_4^-(y) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} IC_4^-(z) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} IC_2(x{+}y) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$IC_2(x{-}y) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} IC_2(x{+}z) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} IC_2(x{-}z) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$IC_2(y+z) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} IC_2(y-z) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

And the projection operator obtained by Equation 23 is:

$$P^{T_1^-} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix},$$

and it can be immediately seen, that the representation is reducible and that there are 3 linearly independent eigenvectors, namely $(1,-1,0,0,0,0)$, $(0,0,1,-1,0)$, $(0,0,0,0,1,-1)$. This means, that the field combinations, that belong to the vector will transform irreducibly under the group O_h:

$$\psi_x^{T_1^-} = M_1(\vec{x})M_2(-\vec{x}) - M_1(-\vec{x})M_2(\vec{x}), \tag{40}$$

$$\psi_y^{T_1^-} = M_1(\vec{y})M_2(-\vec{y}) - M_1(-\vec{y})M_2(\vec{y}), \tag{41}$$

$$\psi_z^{T_1^-} = M_1(\vec{z})M_2(-\vec{z}) - M_1(-\vec{z})M_2(\vec{z}). \tag{42}$$

6 Decomposition of T_1^- of O_h in C_{4v}

For representation purposes, the decomposition of the T_1^- of O_h in C_{4v} can be done. This means, that we take the operations that belong both to O_h and C_{4v} and multiply their characters in the sense of Section 4. Such a decomposition will not give full information on which plane waves are present in a given irreducible representation, however in this special case it will give $l = 1$ partial wave decomposition in C_{4v}; this is due to the fact, that $l = 1$ partial wave was only in the T_1^- irreducible representation:

$$T_1^-(O_h) = A_1(C_{4v}) \oplus E(C_{4v}). \tag{43}$$

Generally the entire series would need to be decomposed and this would no longer be beneficial.

6.1 Basis of A_1 irreducible representation

There is a way to obtain the basis of the irreducible representation of a subgroup of O_h by knowing the transformations in O_h. Specifically the method goes somewhat like: for a given subgroup of O_h take the transformations that belong to the subgroup, but are defined in the O_h irreducible representation. The matrices of this representation that correspond to the subgroup form a subduced representation [5], which is reducible. However there is a benefit; by taking this subduced representation, then sum the matrices in a given class to obtain a new matrix. By finding the matrix that diagonalizes this sum, the matrix that reduces the subduced representation has been found.

The basis for the irreducible basis in O_h is $\psi_1 - \psi_2$, $\psi_3 - \psi_4$, $\psi_5 - \psi_6$. We write the $C_4^{\pm}$ in this irreducible basis:

$$C_4^+(\psi_1 - \psi_2) = \psi_3 - \psi_4, \tag{44}$$

$$C_4^+(\psi_3 - \psi_4) = -(\psi_1 - \psi_2), \tag{45}$$

$$C_4^+(\psi_5 - \psi_6) = \psi_5 - \psi_6, \tag{46}$$

$$C_4^-(\psi_1 - \psi_2) = -(\psi_3 - \psi_4), \tag{47}$$

$$C_4^-(\psi_3 - \psi_4) = \psi_1 - \psi_2, \tag{48}$$

$$C_4^-(\psi_5 - \psi_6) = \psi_5 - \psi_6, \tag{49}$$

which can be written in matrix form:

$$C_4^+ = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, C_4^- = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The sum is obviously:

$$C_4^+ + C_4^- = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

This matrix is diagonalized trivialy. From this follow, that after aplying the matrix, that diagonalizes it, to the the basis we obtain a irreducible representation of the group C_{4v}. The basis vector $\psi_5 - \psi_6$ transforms as the A_1 irreducible representation of C_{4v}:

$$A_1: \quad \psi^{A_1} = M_1(\vec{z})M_2(-\vec{z}) - M_1(-\vec{z})M_2(\vec{z}) \tag{50}$$

7 Conclusion

The seminar describes how the symmetries of a finite box affect partial waves present in fields that are used in lattice QCD simulations. The general procedure of obtaining fields, that will couple only to minimal amount of partial waves is presented and a complete example made. Fields obtained from this procedures can be used effectively to determine which states occur at which energy. In fact this procedure is crucial to reliably determine a state when doing hadron spectroscopy from lattice QCD. It is worth noting, that although the above procedure was done for the case of two meson fields, it holds also for baryon fields, however there the double cover of O_h needs to be considered and this introduces some technical difficulties; O_h is already a big group, however its double cover is still larger. The seminar also demonstrates how once a irreducible basis in a larger group is already obtained how to determine some parts of a basis for a smaller group as a freebie.

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