

## **Supplement 2: Continuous Groups of $O(N)$ , $SO(N)$ and $SU(N)$**

Symmetry is one of the guiding principles in physics, and group theory that describes symmetries in nature plays an essential role in our studies of quantum field theory. In general, symmetries can range from external to internal, from global to local, from finite to infinite, and from ordinary to supersymmetry. Here we discuss basic properties of the continuous groups of  $O(N)$ ,  $SO(N)$ , and  $SU(N)$ .

### • Representations of $O(2)$ , $SO(2)$ , and $U(1)$

We begin with the simplest nontrivial example of  $O(2)$ , which corresponds to rotations in two dimensions. Our objective is to construct the irreducible representations of  $O(2)$ , and we note that the length  $(x^2 + y^2)^{1/2}$  is invariant under a rotation about the origin if  $(x, y)$  denotes a point on the plane. If we rotate the plane through an angle  $\theta$ , then the coordinates  $(x', y')$  of the same point in the new system become

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \quad (\text{S2.1})$$

which can be abbreviated by:

$$(x')^i = O^{ij}(\theta) x^j, \quad (\text{S2.2})$$

with  $x^1 = x$ ,  $x^2 = y$ . Here we note that for the rotation group, it makes no difference whether the index is placed as a superscript or as a subscript. For small angles, EQ. (S2.2) is reduced to

$$\delta x = \theta y; \quad \delta y = -\theta x \quad \rightarrow \quad \delta x^i = \theta \varepsilon^{ij} x^j, \quad (\text{S2.3})$$

where  $\varepsilon^{ij}$  is antisymmetric and  $\varepsilon^{12} = -\varepsilon^{21} = 1$ . These rotation matrices  $O(\theta)$  form a group, and the inverse of any rotation is given by  $O^{-1}(\theta) = O(-\theta)$ :

$$O(\theta) O(-\theta) = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

In addition, we can prove associativity of these matrices because the matrix multiplication is associative.

The fact that these matrices preserve the invariant length imposes restrictions on them. If we consider a rotation on the invariant distance, we find that

$$\begin{aligned} (x')^i (x')^i &= O^{ij}(\theta) x^j O^{ik}(\theta) x^k = x^j O^{ij}(\theta) O^{ik}(\theta) x^k = x^j x^j \\ &\rightarrow [O^{ij}(\theta) O^{ik}(\theta)] = \delta^{jk} \quad \leftrightarrow \quad O^T O = I. \end{aligned} \quad (\text{S2.4})$$

Therefore we can obtain the inverse of a matrix by simply taking its transpose, and the unit matrix  $I$  is called the *metric* of the group.

The rotation group  $O(2)$  is called the *orthogonal group* in two dimensions, and can be defined as a set of all real two-dimensional orthogonal matrices. In general, any orthogonal matrix with determinant 1 can be expressed as the exponential of a single antisymmetric matrix  $\tau$ .

$$O(\theta) = e^{\theta \tau} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} (\theta \tau)^n, \quad (\text{S2.5})$$

where

$$\tau = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \quad (\text{S2.6})$$

Noting that the transpose of  $e^{\theta\tau}$  is  $e^{-\theta\tau}$ , we find that

$$O^T = (e^{\theta\tau})^T = e^{-\theta\tau} = O^{-1}. \quad (\text{S2.7})$$

In addition, we can expand and rewrite EQ. (S2.5) into the sum of two infinite series, so that:

$$O(\theta) = e^{\theta\tau} = \left[ 1 + \sum_{n=1}^{\infty} \frac{1}{2n!} (-\theta^2)^n \right] + \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} (-\theta^2)^n \tau = \cos\theta I + \tau \sin\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \quad (\text{S2.8})$$

If we take the determinant of both sides of EQ. (S2.4), we find that

$$\det(OO^T) = \det(O)\det(O^T) = [\det(O)]^2 = 1.$$

Thus, the determinant of  $O$  is equal to  $\pm 1$ . If we take  $\det O = 1$ , the resulting subgroup is called  $SO(2)$ , the special orthogonal matrices in two dimensions. On the other hand, the subgroup with  $\det O = -1$  consists of elements of  $SO(2)$  multiplied by the matrix:

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

which corresponds to a parity transformation  $x \rightarrow x$  and  $y \rightarrow -y$  in two dimensions.

The two-dimensional matrices  $O^{ij}$  associated with  $O(2)$  satisfies the following multiplication rule:

$$O^{ij}(\theta)O^{jk}(\theta') = O^{ik}(\theta + \theta'), \quad (\text{S2.9})$$

In fact, any matrix representation  $D(\theta)$  (not necessarily orthogonal or not even  $2 \times 2$  in size) that satisfies the multiplication rule

$$D(\theta)D(\theta') = D(\theta + \theta'); \quad D(\theta) = D(\theta + 2\pi) \quad (\text{S2.10})$$

forms a representation of  $O(2)$ .

For most applications of group theory to quantum mechanics and quantum field theory, we are primarily interested in the transformation properties of fields. To understand how a field  $\varphi(x)$  transforms under rotations, we introduce an operator  $L$  such that

$$L \equiv -i\epsilon^{ij}x^i \frac{\partial}{\partial x_j} = -i(x^1\partial^2 - x^2\partial^1). \quad (\text{S2.11})$$

We also define  $U(\theta)$  by  $L$  as follows:

$$U(\theta) \equiv e^{-i\theta L}. \quad (\text{S2.12})$$

Using EQs. (S2.11) and (S2.12), we define a scalar field as a field that transforms under  $SO(2)$  according to:

$$\text{Scalar: } U(\theta)\varphi(x)U^{-1}(\theta) = \varphi(x'). \quad (\text{S2.13})$$

We can also define a vector field  $\varphi^i(x)$ , where the additional index also transforms under rotation according to the following relation:

$$\text{Vector: } U(\theta)\varphi^i(x)U^{-1}(\theta) = O^{ij}(-\theta)\varphi^j(x'). \quad (\text{S2.14})$$

We can further generalize the above formula to include the transformation properties of arbitrary fields. If we define  $\varphi^A(x)$  as an arbitrary field transforming under certain representation of  $SO(2)$  labeled by some index  $A$ , then the field transforms as:

$$U(\theta)\varphi^A(x)U^{-1}(\theta) = D^{AB}(-\theta)\varphi^B(x'), \quad (\text{S2.15})$$

where  $D^{AB}$  is a representation of the group, which can be either reducible or irreducible.

Generally speaking, the basic fields of physics transform as irreducible representations of the Lorentz and Poincaré groups, so we are interested in finding all irreducible representations of the group in question. For the  $O(N)$  group, the complete set of finite dimensional representations comes in two types of representations, the tensors and the spinors. Here we consider specific examples of generating higher tensor representations of  $O(2)$ . A simple way is to multiply several vectors together and to observe the corresponding transformation. For instance, the product  $A^i B^j$  transforms as follows:

$$(A^i B^j) = [O^{ii}(\theta)O^{jj}(\theta)](A^i B^j), \quad (\text{S2.16})$$

where the matrix  $O^{ii}(\theta)O^{jj}(\theta)$  forms a representation of  $SO(2)$ , which has the same multiplication rule as  $O(2)$ , but it acts upon a  $(2 \times 2)$  dimensional space. We refer any object (such as  $A^i B^j$  given above) that transforms like the product of several vectors as a tensor.

In general, a tensor  $T^{ijk\dots}$  under  $O(2)$  is an object that transforms like the product of a series of ordinary vectors:

$$\text{Tensor: } (T')^{i_1, i_2, \dots} = O^{i_1, i_1} O^{i_2, i_2} \dots T^{i_1, i_2, \dots} \quad (\text{S2.17})$$

The transformation of  $T^{i_1, i_2, \dots}$  is identical to that of the product  $x^i x^j x^k \dots$ . This product forms a representation of  $O(2)$  because the following transformation matrix has the same multiplication rule as  $SO(2)$ :

$$O^{i_1, i_2, \dots, i_N; j_1, j_2, \dots, j_N}(\theta) = O^{i_1, j_1}(\theta) O^{i_2, j_2}(\theta) \dots O^{i_N, j_N}(\theta). \quad (\text{S2.18})$$

The tensors that we can generate by taking products of vectors are generally reducible. To extract the irreducible representations from these tensors, we need to take appropriate symmetric and antisymmetric combinations of the indices. A convenient method is to use two tensors that are actually constants under  $O(2)$ :  $\delta^{ij}$  and  $\varepsilon^{ij}$ , where the latter is the antisymmetric constant tensor. To see that  $\delta^{ij}$  and  $\varepsilon^{ij}$  are indeed tensors, we note that

$$\delta^{i'j'} = O^{ii} O^{jj} \delta^{ij}, \quad (\text{S2.19})$$

$$\varepsilon^{i'j'} = O^{ii} O^{jj} \varepsilon^{ij}. \quad (\text{S2.20})$$

Clearly EQ. (S2.19) is just the definition of an orthogonal matrix, and therefore  $\delta^{ij}$  is an invariant tensor. On the other hand, EQ. (S2.20) is just the definition of the determinant of the  $O$  matrix, which is equal to 1 under  $SO(2)$ . We also mention that  $\varepsilon^{ij}$  transforms like a tensor only if the determinant of the  $O$  matrix is +1, so that  $\varepsilon^{ij}$  is sometimes called a *pseudotensor*. The pseudotensors pick up an extra minus sign when they are transformed under parity transformation.

Using the two constant tensors  $\delta^{ij}$  and  $\varepsilon^{ij}$ , we can immediately contract the tensor  $A^i B^j$  to form two scalar combinations:

$$A^i \delta^{ij} B^j = A^i B^i \quad \text{and} \quad A^i \varepsilon^{ij} B^j = A^1 B^2 - A^2 B^1.$$

The processes of symmetrizing and anti-symmetrizing all possible tensor indices to find the irreducible representations are also aided by the following identities:

$$\varepsilon^{ij} \varepsilon^{kl} = \delta^{ik} \delta^{jl} - \delta^{il} \delta^{jk}, \quad (\text{S2.21})$$

$$\varepsilon^{ij} \varepsilon^{jk} = -\delta^{ik}. \quad (\text{S2.22})$$

Finally, we consider expressing  $O(2)$  in another formulation. If we take a complex field  $\varphi = \varphi_1 + i\varphi_2$  and transform it under a unitary matrix  $U(\theta)$  such that

$$\varphi' = U(\theta)\varphi = e^{i\theta}\varphi, \quad (\text{S2.23})$$

the set of all one-dimensional unitary matrices  $U(\theta)$  defines a  $U(1)$  group, and the combined transformation

$$e^{i\theta} e^{i\theta'} = e^{i(\theta+\theta')} \quad (\text{S2.24})$$

satisfies the same multiplication rules as  $O(2)$ . Hence, there is a local correspondence between  $O(2)$  and  $U(1)$ , although they are defined in two different spaces:

$$SO(2) \leftrightarrow U(1), \quad e^{\tau(\theta)} \leftrightarrow e^{i\theta}. \quad (\text{S2.25})$$

### • Representations of $SO(3)$ and $SU(2)$

The continuous group  $O(2)$  consists of elements that are commutative with each other, and therefore is an Abelian group. In contrast, the elements in the three-dimensional orthogonal group  $O(3)$  that involve invariant distance  $(x^2 + y^2 + z^2)^{1/2}$  under three-dimensional rotations do not necessarily commute with each other. Such a group is known as a non-Abelian group. The transformation of coordinates under  $O(3)$  symmetry can be described by a set of  $(3 \times 3)$  real and orthogonal matrices, such that

$$(x')^i = O^{ij} x^j \quad \text{and} \quad \sum_{i=1}^3 [(x')^i]^2 = \sum_{i=1}^3 (O^{ij} x^j)^2 = \sum_{j=1}^3 (x^j)^2.$$

The condition of orthogonality reduces the number of independent elements to 3 in the  $O(3)$  group. Specifically, any element of the  $O(3)$  group can be expressed as the exponential of an anti-symmetric matrix

$$O = \exp\left(-i \sum_{j=1}^3 \theta^j \tau^j\right), \quad (\text{S2.26})$$

where  $\tau^j$  has purely imaginary elements. There are 3 independent anti-symmetric  $(3 \times 3)$  matrices in the  $O(3)$  group, which correspond to the correct counting of independent degrees of freedom. Therefore  $O(3)$  is a three-dimensional Lie group parameterized by three angles.

The three anti-symmetric matrices  $\tau^j$  can be explicitly written as:

$$\tau^1 = \tau^x = -i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}; \quad \tau^2 = \tau^y = -i \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}; \quad \tau^3 = \tau^z = -i \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{S2.27})$$

The set of matrices in EQ. (S2.27) can be succinctly represented by the anti-symmetric tensor  $\varepsilon^{ijk}$  as follows:

$$(\tau^i)^{jk} = -i\varepsilon^{ijk}, \quad (\text{S2.28})$$

where  $\varepsilon^{123} = +1$ , and the anti-symmetric matrices obey the following properties:

$$[\tau^i, \tau^j] = i\varepsilon^{ijk}\tau^k. \quad (\text{S2.29})$$

The relation in EQ. (S2.29) is an example of a *Lie algebra*, and the constants  $\varepsilon^{ijk}$  appearing in the algebra are the *structure constants* of the algebra. A complete determination of the structure constants specifies the algebra and also the group itself.

For small rotation angles  $\theta^i$ , the transformation law of the  $O(3)$  group can be written as:

$$\delta x^i = \varepsilon^{ijk}\theta^k x^j. \quad (\text{S2.30})$$

Similar to EQ. (S2.11) for the  $O(2)$  group, we introduce the operators:

$$L^i \equiv -i\varepsilon^{ijk}x^j\partial^k. \quad (\text{S2.31})$$

It can be shown that the commutation relations of the operators  $L^i$  satisfy those of the  $SO(3)$  group. Using  $L^i$  defined in EQ. (S2.31), we can construct the transformation matrices  $U(\theta^i)$ :

$$U(\theta^i) \equiv \exp(-i\theta^i L^i). \quad (\text{S2.32})$$

Hence, the scalar and vector fields in  $O(3)$  transform as follows:

$$\text{Scalar: } U(\theta^k)\varphi(x)U^{-1}(\theta^k) = \varphi(x'), \quad (\text{S2.33})$$

$$\text{Vector: } U(\theta^k)\varphi^i(x)U^{-1}(\theta^k) = (O^{-1})^{ij}(\theta^k)\varphi^j(x'). \quad (\text{S2.34})$$

For higher tensor fields, we can decompose a reducible tensor into the irreducible fields by taking appropriate symmetric and anti-symmetric combinations of the indices. Similar to our previous discussions of the  $O(2)$  group, the irreducible representations of the  $O(3)$  group can be extracted by using two constant tensors  $\delta^{ij}$  and  $\varepsilon^{ijk}$ . Moreover, in carrying out the reduction, it is helpful to know the following identities:

$$\varepsilon^{ijk}\varepsilon^{lmn} = \delta^{il}\delta^{jm}\delta^{kn} - \delta^{il}\delta^{jn}\delta^{km} + \delta^{im}\delta^{jn}\delta^{kl} - \delta^{im}\delta^{jl}\delta^{kn} + \delta^{in}\delta^{jl}\delta^{km} - \delta^{in}\delta^{jm}\delta^{kl}, \quad (\text{S2.35})$$

$$\varepsilon^{ijk}\varepsilon^{klm} = \delta^{il}\delta^{jm} - \delta^{im}\delta^{jl}. \quad (\text{S2.36})$$

Finally, as in the case of the  $O(2)$  group, we can also find a relationship between  $O(3)$  and a unitary group. Consider the set of all unitary ( $2 \times 2$ ) matrices with unit determinant. These matrices form a group known as  $SU(2)$ , the special unitary group in two dimensions, and each matrix contains three independent elements. Since each unitary matrix  $U$  with unit determinant can be expressed in terms of the exponential of a Hermitian matrix  $H$ :

$$U = e^{iH},$$

it is convenient to use the three Hermitian Pauli matrices to represent the elements of  $SU(2)$ . That is, any element in  $SU(2)$  can be expressed as:

$$U = \exp(-i\theta^i\sigma^i/2), \quad (\text{S2.37})$$

where the Pauli matrices  $\sigma^i$  are given by:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (\text{S2.38})$$

and  $\sigma^i$  satisfy the relationship:

$$\left[ \frac{\sigma^i}{2}, \frac{\sigma^j}{2} \right] = i\epsilon^{ijk} \frac{\sigma^k}{2}. \quad (\text{S2.39})$$

The algebra of  $SU(2)$  in EQ. (S2.39) is the same as that of  $SO(3)$  in EQ. (S2.29), so that

$$SO(3) \sim SU(2): \quad \exp(-i\tau^j \theta^j) \leftrightarrow \exp(-i\sigma^j \theta^j / 2) = \cos(\theta/2)I - i(\sigma^k n^k) \sin(\theta/2), \quad (\text{S2.40})$$

where  $\theta^i = n^i \theta$  and  $\sum_i (n^i)^2 = 1$ . Although the representations in  $SO(3)$  are real ( $3 \times 3$ ) orthogonal matrices and those in  $SU(2)$  are ( $2 \times 2$ ) unitary matrices, they in fact obey the same multiplication law. We therefore expect that the three-dimensional vectors  $(x, y, z)$  can be expressed in terms of the spinors. Indeed, if we define

$$h(\vec{x}) = \vec{\sigma} \cdot \vec{x} = \begin{pmatrix} z & x - iy \\ x + iy & z \end{pmatrix}, \quad (\text{S2.41})$$

we find that the  $SU(2)$  transformation:

$$h' = U h U^{-1} \quad (\text{S2.42})$$

is equivalent to the  $SO(3)$  transformation:

$$\vec{x}' = \vec{O} \cdot \vec{x}. \quad (\text{S2.43})$$

### • Representations of $SO(N)$

Having considered the more familiar cases of  $SO(2)$  and  $SO(3)$  groups, we are ready to generalize to the  $SO(N)$  group for any positive integer  $N$ . The special orthogonal group  $SO(N)$  consists of all  $(N \times N)$  real matrices  $O$  that are orthogonal (*i.e.*,  $O^T O = 1$ ) and have unit determinant (*i.e.*,  $\det O = 1$ ). The group  $SO(N)$  consists of rotations in  $N$ -dimensional Euclidean space, and its fundamental representation can be given by the  $N$ -component vector  $\vec{v} = \{v^j, j=1, \dots, N\}$ , which transforms under the action of the group element  $O$  according to the following:

$$v^i \rightarrow v'^i = O^{ij} v^j. \quad (\text{S2.44})$$

Similar to our earlier discussions on the  $SO(2)$  and  $SO(3)$  groups, we define tensors as objects that transform like the product of vectors. For instance, the tensor  $T^{ijk}$  transforms according to

$$T^{ijk} \rightarrow T'^{ijk} = O^{il} O^{jm} O^{kn} T^{lmn}. \quad (\text{S2.45})$$

We can envision  $T^{ijk}$  as a collection of  $N^3$  objects being acted upon by an  $(N^3 \times N^3)$  matrix. The number of objects in a tensor is called the dimension of the representation.

In general, we can reduce a tensor representation into symmetric and anti-symmetric representations. Let's consider a simple example:

$$T^{ij} \rightarrow T'^{ij} = O^{il} O^{jm} T^{lm}. \quad (\text{S2.46})$$

We can form the symmetric ( $S^{ij}$ ) and anti-symmetric ( $A^{ij}$ ) combinations as follows:

$$S^{ij} \equiv \frac{1}{2}(T^{ij} + T^{ji}), \quad A^{ij} \equiv \frac{1}{2}(T^{ij} - T^{ji}). \quad (\text{S2.47})$$

The symmetric combination  $S^{ij}$  transforms into  $O^{il}O^{jm}S^{lm}$ , and the anti-symmetric combination  $A^{ij}$  transforms into  $O^{il}O^{jm}A^{lm}$ . Therefore, the  $N^2$  objects contained in  $T^{ij}$  split into two sets, with  $N(N+1)/2$  contained in  $S^{ij}$  that transform among themselves, and  $N(N-1)/2$  contained in  $A^{ij}$  that also transform among themselves. Clearly the representations furnished by  $T^{ij}$  are reducible. Moreover, given symmetric tensors  $S^{ij}$ , we can define the combination  $T \equiv \sum_{ij} \delta^{ij} S^{ij}$ , which is known as the trace. It follows that

$$\begin{aligned} T \rightarrow T' &= \sum_{ij} \delta^{ij} S'^{ij} = \sum_{lm} \sum_{ij} \delta^{ij} O^{il} O^{jm} S^{lm} = \sum_{lm} \sum_{ij} (O^T)^{li} \delta^{ij} O^{jm} S^{lm} = \sum_{lm} \sum_i (O^T)^{li} O^{im} S^{lm} \\ &= \sum_{lm} \delta^{lm} S^{lm} = T. \end{aligned}$$

In other words, the trace is invariant under rotation. We can therefore subtract the trace from the symmetric tensors, so that the  $[N(N+1)/2 - 1]$  traceless symmetric tensors  $Q^{ij}$  transform among themselves, where

$$Q^{ij} \equiv S^{ij} - \frac{1}{N} \delta^{ij} T.$$

Hence, given two vectors, we can form a tensor and decompose it into a symmetric traceless combination, a trace, and an anti-symmetric tensor. This process can be expressed as:

$$N \otimes N = \left[ \frac{1}{2} N(N+1) - 1 \right] \oplus 1 \oplus \left[ \frac{1}{2} N(N-1) \right]. \quad (\text{S2.48})$$

Specifically, for the  $SO(3)$  group, we have  $3 \otimes 3 = 5 \oplus 1 \oplus 3$ . We can think of EQ. (S2.48) as the direct product of two states, both of angular momentum  $L = 1$ , which is subsequently reduced to  $L = 0, 1$ , and  $2$ .

The condition  $\det O = 1$  for the  $SO(N)$  group can be expressed in terms of the anti-symmetric symbol  $\varepsilon^{123\dots N}$  as follows:

$$\varepsilon^{i_1 i_2 \dots i_N} O^{i_1 1} O^{i_2 2} \dots O^{i_N N} = 1 \rightarrow \varepsilon^{i_1 i_2 \dots i_N} O^{i_1 j_1} O^{i_2 j_2} \dots O^{i_N j_N} = \varepsilon^{j_1 j_2 \dots j_N}. \quad (\text{S2.49})$$

We can multiply EQ. (S2.49) repeatedly to generate more identities. For instance, for  $N = 3$ , we find that

$$\varepsilon^{i_1 i_2 i_3} O^{i_1 j_1} O^{i_2 j_2} = \varepsilon^{j_1 j_2 j_3} (O^T)^{j_3 j_3}. \quad (\text{S2.50})$$

Given the orthogonality condition  $O^T O = 1$ , the number of independent elements in each member of the  $O(N)$  group is  $N^2$  minus the  $N(N+1)/2$  orthogonality constraints. Hence, there are  $N(N-1)/2$  independent elements, which is exactly the number of independent anti-symmetric representations. Consequently, any orthogonal matrix can be generally parameterized as follows:

$$O = \exp \left( -i \sum_{j=1}^{N(N-1)/2} \theta^j \tau^j \right), \quad (\text{S2.51})$$

where  $\tau^j$  are linearly independent antisymmetric matrices with purely imaginary elements, which are known as the *generators* of the group, and  $\theta^j$  are the rotation angles or the *parameters* of the group. Having defined the antisymmetric generators, we can represent the algebra of the group according to the following:

$$[\tau^i, \tau^j] = i f^{ijk} \tau^k, \quad (\text{S2.52})$$

where  $f^{ijk}$  are the structure constants of the group. As discussed before, the structure constants can be thought of as a representation of the algebra.

For any arbitrary  $N$ , we can in principle find an exact form for the structure constants by defining the generators  $M^{ij}$  of  $O(N)$ . For instance, if we define:

$$(M^{ij})_{ab} = i(\delta_a^i \delta_b^j - \delta_a^j \delta_b^i), \quad (\text{S2.53})$$

where the subscripts  $a$  and  $b$  refer to the  $a$ th row and the  $b$ th column of the anti-symmetric matrix  $M^{ij}$ , we can commute these matrices and obtain the following general relation:

$$[M^{ij}, M^{kl}] = -i(\delta^{ik} M^{jl} - \delta^{jk} M^{il} + \delta^{jl} M^{ik} - \delta^{il} M^{jk}). \quad (\text{S2.54})$$

If we choose a specific set of generators  $J^{ij}$

$$J^{ij} \equiv -i(x^i \partial^j - x^j \partial^i) \quad (\text{S2.55})$$

such that the operator  $U(\theta^{ij})$  can be constructed as:

$$U(\theta^{ij}) \equiv \exp(-i\theta^{ij} J^{ij}) \quad (\text{S2.56})$$

with  $\theta^{ij}$  being anti-symmetric, we find that the generators  $J^{ij}$  indeed satisfy the algebra in EQ. (S2.54), and that they can be thought of as the effective ‘‘angular momentum’’ representation in  $O(N)$ . On the other hand, if we choose our generators such that

$$M^{ij} \equiv \frac{i}{4}[\Gamma^i, \Gamma^j], \quad (\text{S2.57})$$

where  $\Gamma^i$  represent  $N$  objects that satisfy the Clifford algebra:

$$\{\Gamma^i, \Gamma^j\} = \Gamma^i \Gamma^j + \Gamma^j \Gamma^i = 2\delta^{ij}, \quad (\text{S2.58})$$

we find that the new generators also satisfy the general relation in EQ. (S2.54), and we have constructed the *spinor representation* of the  $SO(N)$  group.

In general, by examining the algebra of given groups, we can determine whether certain groups are locally isomorphic to each other. We have seen earlier that the following relations hold:

$$SO(2) \sim U(1); \quad SO(3) \sim SU(2).$$

Moreover, we note that the Lorentz group can be expressed by  $SO(3,1)$ , which is directly related to the  $SO(4)$  group in the Euclidean space. In fact, it can be shown that

$$SO(4) \sim SO(3) \otimes SO(3) \text{ and } SO(3,1) \sim SU(2) \otimes SU(2).$$

For more detailed discussion on properties of the Lorentz group, you may refer to Supplement\_3 notes. In the following we consider the  $SU(N)$  group for general  $N$ .

• **Representations of  $SU(N)$**

The  $SU(N)$  symmetries are of particular importance to the standard model that involves symmetries of  $U(1) \otimes SU(2) \otimes SU(3)$  and the Grand Unified Theory that considers  $SU(5)$  or  $O(10)$  symmetry. The special unitary group  $SU(N)$  consists of all  $(N \times N)$  matrices  $U$  that are unitary:

$$U^\dagger U = 1, \tag{S2.59}$$

and have unit determinant:

$$\det U = 1. \tag{S2.60}$$

The defining representation of  $SU(N)$  consists of  $N$  objects  $\varphi^j$  ( $j=1, \dots, N$ ) that transform under the symmetry operation of the group element  $U$  according to

$$\varphi^i \rightarrow \varphi'^i = U_j^i \varphi^j, \tag{S2.61}$$

where we have denoted the element in the  $i$ th row and the  $j$ th column of the group element by  $U_j^i$ . If we take the complex conjugate of EQ. (S2.61) and define that the object  $\varphi_j$  transforms like  $\varphi^{*j}$ , we obtain

$$\varphi^{*i} \rightarrow (U_j^i)^* \varphi^{*j} = (U^\dagger)_i^j \varphi^{*j} \Leftrightarrow \varphi_i \rightarrow \varphi'_i = (U^\dagger)_i^j \varphi_j. \tag{S2.62}$$

We can also construct tensors in  $SU(N)$ . For instance, the tensor  $\varphi_k^{ij}$  transforms like the product  $\varphi^i \varphi^j \varphi_k$ :

$$\varphi_k^{ij} \rightarrow \varphi_k'^{ij} = U_l^i U_m^j (U^\dagger)_k^n \varphi_n^{lm}. \tag{S2.63}$$

Here  $\varphi^j$  is called a covariant vector and  $\varphi_j$  a contravariant vector. In general, a tensor  $\varphi_{j_1, j_2, \dots, j_n}^{i_1, i_2, \dots, i_m}$  with  $m$  upper indices and  $n$  lower indices is defined to transform as if it is equal to the product of  $m$  covariant vectors and  $n$  contravariant vectors. Such a tensor is sometimes denoted as  $(m, n)$ . It is also customary to denote a tensor  $(m, 0)$  simply as  $m$ , and the tensor  $(0, n)$  as  $n^*$ . Moreover, we can rewrite the condition in EQ. (S2.59) into the following:

$$(U^\dagger)_i^k U_k^j = \delta_i^j. \tag{S2.64}$$

To take the trace of an object, we consider  $\delta_j^k \varphi_k^{ij} \equiv \varphi_j^{ij}$ , which transforms as

$$\varphi_j^{ij} \rightarrow \varphi_j'^{ij} = U_l^i U_m^j (U^\dagger)_j^n \varphi_n^{lm} = U_l^i \varphi_m^{lm}. \tag{S2.65}$$

In other words,  $\varphi_j^{ij}$ , the trace of  $\varphi_k^{ij}$ , denotes  $N$  objects that transform into linear combinations of each other in the same way as the covariant vector  $\varphi^i$ . Hence, given a tensor in  $SU(N)$ , we can always subtract out its trace, similar to the case in  $SO(N)$ . In addition, we can always take a tensor  $\varphi_k^{ij}$  to be either symmetric or anti-symmetric under the exchange of  $i$  and  $j$  and also to be traceless. Thus, the symmetric traceless tensor  $\varphi_k^{ij}$  furnishes a representation with dimension  $[N^2(N+1)/2 - N]$ , and the anti-symmetric traceless tensor  $\varphi_k^{ij}$  furnishes a representation with dimension  $[N^2(N-1)/2 - N]$ . Moreover, we note that the dimension for the covariant vector  $\varphi^i$  is  $N$ , for the antisymmetric tensor  $\varphi^{ij}$  is  $[N(N-1)/2]$ , for the symmetric tensor  $\varphi^{ij}$  is  $[N(N+1)/2]$ , for the traceless tensor  $\varphi_i^i$  is  $(N^2 - 1)$ , and for the tensor  $\varphi_k^{ij}$  anti-symmetric in the upper indices is  $[N^2(N-1)/2 - N]$ . If we take  $SU(5)$  for example, we find that the dimensions for the

representations  $\varphi^i$ ,  $\varphi^{ij}$  (anti-symmetric),  $\varphi^{ij}$  (symmetric),  $\varphi_j^i$  (traceless), and  $\varphi_k^{ij}$  (anti-symmetric in the upper indices) are 5, 10, 15, 24, and 45, respectively.

The representation defined by the traceless tensor  $\varphi_j^i$  is known as the adjoint representation, which, by definition, transforms according to

$$\varphi_j^i \rightarrow \varphi_j^{\prime i} = U_l^i (U^\dagger)_j^n \varphi_n^l = U_l^i \varphi_n^l (U^\dagger)_j^n \Leftrightarrow \varphi \rightarrow \varphi' = U \varphi U^\dagger. \quad (\text{S2.66})$$

From EQ. (S2.66), we note that if  $\varphi$  is hermitian, it remains hermitian after transformation. Moreover, given a hermitian traceless matrix  $X$ ,  $U X U^\dagger$  is also hermitian if  $U$  is an element of  $SU(N)$ .

Similar to the case of  $SO(N)$ , the condition  $\det U = 1$  in EQ. (S2.60) can be written as follows:

$$\varepsilon_{i_1 i_2 \dots i_N} U_1^{i_1} U_2^{i_2} \dots U_N^{i_N} = 1 \quad \& \quad \varepsilon^{i_1 i_2 \dots i_N} U_1^{i_1} U_2^{i_2} \dots U_N^{i_N} = 1. \quad (\text{S2.67})$$

Hence, we have two anti-symmetric tensors  $\varepsilon_{i_1 i_2 \dots i_N}$  and  $\varepsilon^{i_1 i_2 \dots i_N}$  that we can use to raise and lower indices. We can also generalize EQ. (S2.67) into the following identity:

$$\varepsilon_{i_1 i_2 \dots i_N} U_{j_1}^{i_1} U_{j_2}^{i_2} \dots U_{j_N}^{i_N} = \varepsilon_{j_1 j_2 \dots j_N}. \quad (\text{S2.68})$$

If we multiply EQ. (S2.68) by  $(U^\dagger)_{p_N}^{j_N}$  and sum over  $j_N$ , we obtain

$$\varepsilon_{i_1 i_2 \dots p_N} U_{j_1}^{i_1} U_{j_2}^{i_2} \dots U_{j_{N-1}}^{i_{N-1}} = \varepsilon_{j_1 j_2 \dots j_N} (U^\dagger)_{p_N}^{j_N}. \quad (\text{S2.69})$$

We can repeat a similar process to obtain various identities, similar to what we have done for  $SO(N)$  in EQ. (S2.50).

As an example, we consider multiplying an anti-symmetric constant tensor to the representation  $\varphi_k^{ij}$  in  $SU(4)$ . If we define the tensor  $\varphi_{k pq} \equiv \varphi_k^{ij} \varepsilon_{ijpq}$  and use EQ. (S2.69) twice, we find that the tensor  $\varphi_{k pq}$  transforms according to the following:

$$\varphi_{k pq} \equiv \varphi_k^{ij} \varepsilon_{ijpq} \rightarrow \varepsilon_{ijpq} U_l^i U_m^j (U^\dagger)_k^n \varphi_n^{lm} = \varepsilon_{lmst} (U^\dagger)_p^s (U^\dagger)_q^t (U^\dagger)_k^n \varphi_n^{lm} \equiv (U^\dagger)_p^s (U^\dagger)_q^t (U^\dagger)_k^n \varphi_{nst} \quad (\text{S2.70})$$

Given that any unitary matrix with unit determinant can be expressed as  $U = e^{iH}$ , where  $H$  is a hermitian and traceless, we find that there are  $(N^2 - 1)$  linearly independent traceless  $(N \times N)$  hermitian matrices  $T^a$  ( $a = 1, 2, \dots, N^2 - 1$ ) as the generators of  $SU(N)$ . Thus, we can write  $U = \exp(-i\theta^a T^a)$ , where  $\theta^a$  are real numbers and the index  $a$  summed over. We can also define the algebra by considering the anti-hermitian and traceless commutator:

$$[T^a, T^b] = i f^{abc} T^c, \quad (\text{S2.71})$$

where EQ. (S2.71) defines the Lie algebra of  $SU(N)$ , and  $f^{abc}$  are the structure constants. In the case of  $SU(2)$ ,  $f^{abc}$  are simply given by  $\varepsilon^{abc}$ .

For an infinitesimal transformation, we have  $U = \exp(-i\theta^a T^a) \approx 1 - i\theta^a T^a$  so that

$$\varphi^i \rightarrow U_j^i \varphi^j \approx \varphi^i - i\theta^a (T^a)^i_j \varphi^j, \quad (\text{S2.72})$$

which implies that the  $a$ th generator acting on the defining representation gives  $T^a \varphi$ . In addition, if we consider the adjoint representation in EQ. (S2.66), we obtain

$$\varphi \rightarrow \varphi' = U \varphi U^\dagger = (1 - i \theta^a T^a) \varphi (1 - i \theta^a T^a)^\dagger = \varphi - i \theta^a T^a \varphi + \varphi i \theta^a T^a = \varphi - i \theta^a [T^a, \varphi]. \quad (\text{S2.73})$$

Equation (S2.73) implies that the  $a$ th generator operating on the adjoint representation yields  $[T^a, \varphi]$ .

Next, we consider the direct product and the corresponding reduction of tensors in  $SU(N)$ . Given two tensors  $\varphi$  and  $\eta$ , with  $m$  upper and  $n$  lower indices for  $\varphi$  and  $m'$  upper and  $n'$  lower indices for  $\eta$ , respectively, we can construct a tensor  $T$  with  $(m + m')$  upper indices and  $(n + n')$  lower indices that transforms like the product  $\varphi\eta$ , and then reduce  $T$  by various operations introduced earlier. This process is of fundamental importance because we multiply fields together in quantum field theory to construct the Lagrangian. As an example, we consider multiplying the tensor  $5^*$  by  $10$  in  $SU(5)$ , where  $5^*$  corresponds to  $\varphi_k$  and  $10$  refers to anti-symmetric  $\eta^{ij}$  in  $SU(5)$ . To reduce the tensor  $T_k^{ij} = \varphi_k \eta^{ij}$ , we note that we can only separate out the trace  $\varphi_k \eta^{kj}$ , which transforms like  $5$ . Hence, we find that

$$5^* \otimes 10 = 5 \oplus 45. \quad (\text{S2.74})$$

Similarly, if we consider  $10 \otimes 10$  for  $\varphi^{ij} \eta^{kl}$  in  $SU(5)$ , we can write  $\eta^{kl}$  in its equivalent form by lowering the upper two indices with the anti-symmetric constant tensor  $\varepsilon_{mnhkl}$  into three lower indices. Therefore the tensor  $T$  can be expressed as  $T_{mnh}^{ij} = \varphi^{ij} \varepsilon_{mnhkl} \eta^{kl}$ , and its trace is given by  $T_{mij}^{ij}$ , which transforms like  $5^*$ . Moreover, the traceless part of  $T_{mij}^{ij}$  transforms like  $45^*$  according to EQ. (S2.74). Thus, we obtain

$$10 \otimes 10 = 5^* \oplus 45^* \oplus 55^*. \quad (\text{S2.75})$$

Finally, we consider the decomposition of representations in the subgroup of a higher symmetry group. As an example, we note that the three quarks  $u$ ,  $d$ , and  $s$  transform into linear combinations of each other in  $SU(3)$ . On the other hand, a subgroup of the isospin  $SU(2)$  of Heisenberg only transforms  $u$  and  $d$  while leaving  $s$  alone. Therefore the irreducible representation  $3$  of  $SU(3)$  decomposes in  $SU(2)$  into

$$3 \rightarrow 2 \oplus 1. \quad (\text{S2.76})$$

Similarly, for the representation  $3 \otimes 3^*$  in  $SU(3)$ , we have

$$3 \otimes 3^* = 8 \oplus 1, \quad (\text{S2.77})$$

which is further reduced in  $SU(2)$  into:

$$(2 \oplus 1) \otimes (2 \oplus 1) = (3 \oplus 1) \oplus 2 \oplus 2 \oplus 1, \quad (\text{S2.78})$$

so that the traceless tensor  $8$  in  $SU(3)$  is reduced to the following in  $SU(2)$ :

$$8 \rightarrow 3 \oplus 1 \oplus 2 \oplus 2. \quad (\text{S2.79})$$

### • Applications of the $O(3)/SO(3)$ representations to quantum mechanics

As discussed before, the  $SO(3)$  group for proper rotations contains an infinite number of elements and an infinite number of classes. Specifically, the rotations of the same angle about any axis belong to the

same class. Since Hamiltonians with spherical symmetric potentials are invariant under the  $SO(3)$  group, the spherical harmonics  $Y_{lm}(\theta, \phi)$  ( $m = -l, -l + 1, \dots, l - 1, l$ ) that are solutions to the angular part of the Schrödinger equation can be taken as basis functions to generate irreducible representations  $D^{(l)}$  of  $SO(3)$ .

To find the explicit irreducible representation matrices of  $SO(3)$ , we note that a rotation through an angle  $\alpha$  about the  $z$ -axis transforms  $Y_{lm}(\theta, \phi)$  to  $e^{-im\alpha}Y_{lm}(\theta, \phi)$ . Therefore the representation is

$$D^{(l)}(\alpha) = \begin{pmatrix} e^{-il\alpha} & 0 & \dots & 0 \\ 0 & e^{-i(l-1)\alpha} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & e^{il\alpha} \end{pmatrix}, \quad (\text{S2.80})$$

and the corresponding character is

$$\chi^{(l)}(\alpha) = \sum_{m=-l}^l e^{im\alpha} = 1 + 2\cos\alpha + 2\cos(2\alpha) + \dots + 2\cos(l\alpha) = \left[ \frac{\sin\left(\frac{2l+1}{2}\alpha\right)}{\sin\left(\frac{\alpha}{2}\right)} \right]. \quad (\text{S2.81})$$

The characters  $\chi^{(0)}(\alpha)$ ,  $\chi^{(1)}(\alpha)$ ,  $\dots$ ,  $\chi^{(l)}(\alpha)$  constitute a complete set of functions in the interval  $0 \leq \alpha \leq 2\pi$ , and are the only irreducible representations of  $SO(3)$ .

The direct product of the representations of the  $SO(3)$  group can be decomposed into irreducible representations of  $SO(3)$ :

$$D^{(l_1)} \times D^{(l_2)} = \sum_{|l_1-l_2|}^{(l_1+l_2)} D^{(l)}. \quad (\text{S2.82})$$

The rotation-inversion group  $O(3)$  is the direct product of group  $SO(3)$  and group  $I$ . Using EQ. (S2.81), the character table for  $O(3)$  can be obtained and is given below in Table S2.1:

**Table S2.1** Character table of Group  $O(3)$

	$E$	Rotation through $\alpha$	$I$	$I \times$ Rotation through $\alpha$
$D^{(0+)}$	1	1	1	1
$D^{(0-)}$	1	1	-1	-1
$D^{(1+)}$	3	$1 + 2\cos\alpha$	3	$1 + 2\cos\alpha$
$D^{(1-)}$	3	$1 + 2\cos\alpha$	-3	$-(1 + 2\cos\alpha)$
$D^{(l+)}$	$2l + 1$	$\sum_{m=-l}^{+l} e^{im\alpha}$	$2l + 1$	$\sum_{m=-l}^{+l} e^{im\alpha}$
$D^{(l-)}$	$2l + 1$	$\sum_{m=-l}^{+l} e^{im\alpha}$	$-(2l + 1)$	$-\sum_{m=-l}^{+l} e^{im\alpha}$

An example involving the consideration of the direct product of irreducible representations  $D^{(l_1)}$  and  $D^{(l_2)}$  of  $O(3)$  is the case of the non-equivalent electrons in an atom. If two electrons are outside the filled shells of an atom, we may form a direct product presentation of the symmetry group with basis functions  $\psi(1)\varphi(2)$ , where  $\psi(1)$  and  $\varphi(2)$  denote the basis functions of the irreducible representations  $D^{(l_1)}$  and  $D^{(l_2)}$ , respectively. If these two electrons are non-equivalent, *i.e.*, belonging to different  $nl$  subshells, a non-vanishing anti-symmetrized product can be formed for all possible product functions. For instance, consider a  $(2p3p)$  configuration. In the absence of any crystal field, we may express the reducible 9-dimensional representation  $D^{(1)} \times D^{(1)}$  in terms of the irreducible representations of  $O(3)$ , and we find that

$$D^{(1)} \times D^{(1)} = D^{(0)} + D^{(1)} + D^{(2)}.$$

In other words, two non-equivalent  $p$  electrons can couple to produce either an  $s$ - ( $l = 0$ ), a  $p$ - ( $l = 1$ ), or a  $d$ - ( $l = 2$ ) state. Now if we place this atom in a cubic field, the two-electron state will split according to the following consideration of the characters:

$O$	$E$	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$
$D^{(1)}$	3	-1	1	1	0
$D^{(1)} \times D^{(1)}$	9	1	1	1	0
-----					
$\Gamma_1 (A_1)$	1	1	1	1	1
$\Gamma_{12} (E)$	2	2	0	0	-1
$\Gamma_{15} (T_1)$	3	-1	1	-1	0
$\Gamma_{25} (T_2)$	3	-1	-1	1	0

so that  $D^{(1)} \times D^{(1)} = \Gamma_1 + \Gamma_{12} + \Gamma_{15} + \Gamma_{25}$ . In other words, the 9-dimensional product representation in the  $O(3)$  group is reduced to 1 one-dimensional, 1 two-dimensional, and 2 three-dimensional irreducible representations of the cubic  $O$  group. Here we have computed the characters of  $D^{(1)}(\alpha)$  in the cubic  $O$  group by using Table S2.1 and by taking  $\alpha = 0$  for  $E$ ,  $\alpha = \pi$  for  $C_4^2$ ,  $\alpha = \pi/2$  for  $C_4$ ,  $\alpha = \pi/2$  for  $C_2$ , and  $\alpha = 2\pi/3$  for  $C_3$ . (Remember that  $\alpha$  denotes the angle of the symmetry operation axis relative to the  $z$ -axis.) It is worth noting that the situation for two electrons in non-equivalent  $p$  states and under a cubic crystal field environment differs from that for one  $p$ -electron state under a cubic field, because the  $D^{(1)}$  state does not split in a cubic field, as evident from comparing the characters of  $D^{(1)}$  and  $\Gamma_{15}$ .

### Further Readings:

1. Tinkham, "Group Theory and Quantum Mechanics".
2. Zee, "Quantum Field Theory in a Nutshell", Appendix B.
3. Schweber, "An Introduction to Relativistic Quantum Field Theory", Chapter 2.