Quantum Field Theory, Ch2 Supplement

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In classical mechanics or quantum mechanics, we describe the rotation by a linear operator ,operating on the spatial coordinates (x, y, z),represented by a 3×3 matrix,

$$x_i \longrightarrow x'_i = R_{ij} x_j, \qquad \text{where} \qquad RR^T = R^T R = 1$$

For example, rotation by an angle θ around $z-$axis is

$$R_z(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Collection of all these rotations forms the rotation group in 3-dimension, $O(3)$ group. To study the structure of this group, we consider the infinitesmal rotation and write the rotation matrix in the form,

$$R_{ij} = \delta_{ij} + \varepsilon_{ij}, \qquad |\varepsilon_{ij}| \ll 1$$

and

$$x'_i = x_i + \varepsilon_{ij} x_j$$

Orthonality of R,

$$\delta_{jk} = R_{ij} R_{ik} = (\delta_{ij} + \varepsilon_{ij})(\delta_{ik} + \varepsilon_{ik}) \qquad \Longrightarrow \qquad \varepsilon_{jk} = -\varepsilon_{kj}$$

For example, for rotation around $z - axis$,

$$R_z(\theta) \longrightarrow \begin{pmatrix} 1 & \theta & 0 \\ -\theta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \Longrightarrow \qquad \varepsilon_{12} = -\varepsilon_{21} = \theta$$

and

$$x_1' = x_1 + \theta x_2, \qquad x_2' = x_2 - \theta x_1, \qquad x_3' = x_3$$

Consider $f(x_i)$, an arbitrary function of x_i. Under the infinitesimal rotation $R_z(\theta)$, the change in f is

$$f(x) \to f(x_1', x_2', x_3') \approx f(x_1, x_2, x_3) + \theta\left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1}\right) f \cdots$$

Introduce an operator L_3 to represent this change,

$$f(x') = f(x) - i\theta L_3 f(x) + \cdots$$

then

$$L_3 = -i\left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1}\right)$$

For the other rotations,

$$L_1 = -i\left(x_2\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_2}\right), \qquad L_2 = -i\left(x_3\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_3}\right)$$

It is clear that these operators will leave the quadratic form,

$$x_1^2 + x_2^2 + x_3^2$$

invariant.

It is straightforward to show that these operators satisfy

$$[L_i, L_j] = i\varepsilon_{ijk}L_k$$

These are the same as the angular momentum commutation relation.

The operators J_1, J_2, J_3 which satisfy the same commutation relation

$$[J_i, J_j] = i\varepsilon_{ijk}J_k \qquad (1)$$

are called the generators of $R(3)$ and the commutation relations are called the **Lie algebra of** $R(3)$.

Representation of $R(3)$ algebra

Any set of matrices D_1, D_2, D_3 which satisfy the same algebra,

$$[D_i, D_j] = i\varepsilon_{ijk} D_k$$

are called the **representation** of generators J_1, J_2, J_3.
Note that Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

satisfy the commutation relations

$$\left[\frac{\sigma_i}{2}, \frac{\sigma_j}{2}\right] = i\varepsilon_{ijk} \frac{\sigma_k}{2}, \qquad i, j, k = 1, 2, 3$$

So $D_i = \dfrac{\sigma_i}{2}$ is a representation.
To find other representations, define

$$J_\pm = J_1 \pm iJ_2$$

Then

$$[J_\pm, J_3] = \mp J_\pm, \qquad [J_+, J_-] = 2J_3$$

Sincce J_1, J_2, J_3 do not commute, only one of them can be diagonal. Suppose $|m\rangle$ is an eigenstate of J_3 with eigenvalue m,

$$J_3 |m\rangle = m |m\rangle$$

then from these commutation relations,

$$J_3\left(J_+\left|m\right\rangle\right) = (m+1)\left(J_+\left|m\right\rangle\right), \qquad J_3\left(J_-\left|m\right\rangle\right) = (m-1)\left(J_-\left|m\right\rangle\right)$$

Thus J_+ (J_-) is the raising(lowering) operator which increases(decrease) m by one unit. Define total angular momentum operator by

$$J^2 \equiv J_1^2 + J_2^2 + J_3^2 = \frac{1}{2}\left(J_+J_- + J_-J_+ + J_3^2\right) \geq 0 \qquad (2)$$

Then we get

$$\left[J^2, J_i\right] = 0, \qquad \text{for} \quad i = 1, 2, 3$$

and J^2 is called **Casmir operator**, operator which commutes with all the generators in the group.

Choose the states to be eigenstates of J^2, J_3, with eigenvalues, λ, m

$$J^2 \left|\lambda, m\right\rangle = \lambda \left|\lambda, m\right\rangle, \qquad J_3 \left|\lambda, m\right\rangle = m \left|\lambda, m\right\rangle$$

with normalization

$$\left\langle \lambda', m' \mid \lambda, m \right\rangle = \delta_{\lambda\lambda'}\delta_{mm'} \tag{3}$$

From Eq(2) m,is bounded by

$$m^2 \leq \lambda$$

This makes representation matrices finite dimensional. Since $J_\pm \left|\lambda, m\right\rangle$ are eigenstates of J_3 with eigenvalues $m \pm 1$, we can write

$$J_\pm \left|\lambda, m\right\rangle = C_\pm (\lambda, m) \left|\lambda, m \pm 1\right\rangle,$$

Here $C_\pm (\lambda, m)$ are constants to be determined by the normalization conditions in Eq(3). Since $\lambda - m^2 \geq 0$, eigenvalue m^2 is bounded. Thus for largest value of m, say $m = j$, we have

$$J_+ \left|\lambda, j\right\rangle = 0,$$

We can write J^2 as

$$J^2 = \frac{1}{2}\left(J_+J_- + J_-J_+ + J_3^2\right) = J_-J_+ + J_3^2 + J_3$$

Applying this on $\left|\lambda, j\right\rangle$,

$$\left(\lambda - j^2 - j\right)\left|\lambda, j\right\rangle = 0, \qquad \Rightarrow \qquad \lambda = j(j+1)$$

Similarly, for smallest value of m, say $m = j'$,

$$J_- \left|\lambda, j'\right\rangle = 0, \quad \text{and} \quad \lambda = j'\left(j' - 1\right)$$

Combing these two

$$j\,(j+1) = j^{'}\left(j' - 1\right), \quad \Rightarrow \quad j = -j', \;\; \text{or} \quad j' = j + 1$$

The solution $j' = j + 1$ is wrong. Thus we get $j = -j'$. Since J_- decreases value of m by 1 each time,

$$j - j' = 2j = \text{integer}, \qquad \Rightarrow \qquad j \;\; \text{integer or half integer}$$

Use parameter j to label the state

$$J^2 \left|j, m\right\rangle = j\,(j+1) \left|j, m\right\rangle$$

The coefficients $C_{\pm}(\lambda, m)$ can be calculated as follows,

$$J_{+}|j,m\rangle = C_{+}(j,m)|j,m+1\rangle, \qquad \langle j,m|J_{-} = \langle j,m+1|C_{+}^{*}(j,m)$$

$$\langle j,m|J_{-}J_{+}|j,m\rangle = |C_{+}(j,m)|^{2}$$

On the other hand,

$$\langle j,m|J_{-}J_{+}|j,m\rangle = \langle j,m|\left(J^{2}-J_{3}^{2}-J_{3}\right)|j,m\rangle = \left[j(j+1)-m^{2}-m\right] = (j-m)(j+m+1)$$

We can then take

$$C_{+}(j,m) = \sqrt{(j-m)(j+m+1)}$$

Similarly,

$$C_{-}(j,m) = \sqrt{(j+m)(j-m+1)}$$

To summarize, the states $|j,m\rangle$, $m=-j,-j+1,\ldots j-1,j$ form the basis of the irreducible representation characterized by j. These states have the following properties,

$$J^{2}|j,m\rangle = j(j+1)|j,m\rangle, \quad J_{3}|j,m\rangle = m|j,m\rangle \tag{4}$$

$$J_{+}|j,m\rangle = \sqrt{(j-m)(j+m+1)}|j,m+1\rangle, \qquad J_{-}|j,m\rangle = \sqrt{(j+m)(j-m+1)}|j,m-1\rangle \tag{5}$$

Note that we can get the matrix elements of J_1, J_2 by using the relations,

$$J_{1} = \frac{1}{2}(J_{+}+J_{-}), \qquad J_{2} = \frac{1}{2i}(J_{+}-J_{-})$$

Thus for a given value of j, the matrices contructed for J_1, J_2 and J_3 will satisfy the angular momentum algebra given in Eq(1) and they are the irreps of $SU(2)$ group.

Example: $j = \frac{1}{2}, m = \pm\frac{1}{2}$

$$J_3 \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle = \pm\frac{1}{2} \left| \frac{1}{2}, \pm\frac{1}{2} \right\rangle$$

Denote

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Then

$$J_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

From

$$J_+ \left| \frac{1}{2}, \frac{1}{2} \right\rangle = 0, \qquad J_+ \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \left| \frac{1}{2}, \frac{1}{2} \right\rangle$$

we get

$$J_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Also

$$J_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Then

$$J_x = \frac{1}{2}(J_+ + J_-) = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad J_y = \frac{1}{2i}(J_+ - J_-) = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Example : $j = 1, m == -1, 0, 1$
Denote

$$|1,1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |1,-1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

Then from

$$J_3 |1,\pm 1\rangle = \pm |1,\pm 1\rangle, \qquad J_3 |1,0\rangle = 0$$

we get

$$J_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

From

$$J_+ |1,1\rangle = 0, \qquad J_+ |1,0\rangle = \sqrt{2} |1,1\rangle, \qquad J_+ |1,-1\rangle = \sqrt{2} |1,0\rangle$$

we get

$$J_+ = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}$$

and

$$J_- = (J_+)^\dagger = \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

Then

$$J_x = \frac{1}{2}\left(J_+ + J_-\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad J_y = \frac{1}{2i}\left(J_+ - J_-\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

Note that for $j = integer$,

$$J_1 = -i\left(x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2}\right), \qquad J_2 = -i\left(x_3 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3}\right), \qquad J_3 = -i\left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1}\right)$$

Then

$$J_3 x_3 = 0, \qquad J_3 x_1 = i x_2, \qquad J_3 x_2 = -i x_1$$

which implies

$$J_3 (x_1 + i x_2) = (x_1 + i x_2) \qquad J_3 (x_1 - i x_2) = -(x_1 - i x_2)$$

Similarly,

$$J_1 (x_1 + i x_2) = -x_3, \qquad J_1 (x_1 - i x_2) = x_3,$$

Basis for the standard representation are

$$x_+ = -\frac{x_1 + i x_2}{\sqrt{2}}, \qquad x_3, \qquad x_- = \frac{x_1 - i x_2}{\sqrt{2}}$$

SU(2) group

Set of 2×2 unitary matrices with determinant 1 form $SU(2)$ group.
In general, $n \times n$ unitary matrix U can be written as

$$U = e^{iH} \qquad H : n \times n \text{ hermitian matrix}$$

From the identity

$$\det U = e^{iTrH}$$

we get

$$TrH = 0 \qquad if \qquad detU = 1$$

Thus $n \times n$ unitary matrices U can be written in terms of $n \times n$ traceless Hermitian matrices.

Note that Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

is a complete set of 2×2 hermitian traceless matrices. We can use them to describe $SU(2)$ matrices.
Define $J_i = \frac{\sigma_i}{2}$. We can compute the commutators

$$[J_1, J_2] = iJ_3 \quad , \quad [J_2, J_3] = iJ_1 \quad , \quad [J_3, J_1] = iJ_2 \tag{6}$$

This is the *Lie* algebra of $SU(2)$ symmetry. This is exactly the same as the commutation relation of angular momentum in quantum mechanics.

SU(2) and rotation group

Eventhough rotation group $O(3)$ and the unitary group $SU(2)$ are two different groups. It turns out that their structures are almost the same. We will now illustrate this connection.
As we discussed above, the generators of $SU(2)$ group are Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Let $\overrightarrow{r} = (x, y, z)$ be arbitrary vector in R_3 (3 dimensional coordinate space). Define a 2×2 matrix h by

$$h = \vec{\sigma} \cdot \overrightarrow{r} = \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix}$$

This matrix has the following properties;

1. $h^+ = h$
2. $Trh = 0$

$det \ h = -(x^2 + y^2 + z^2)$Let U be a 2×2 unitary matrix with $detU = 1$. Consider the transformation

$$h \rightarrow h' = UhU^\dagger$$

The new matrix h' will have the same properties as h;

1. $h'^+ = h'$
2. $Trh' = 0$

3. $\det h' = \det h$

Properties (1)&(2) imply that h' can also be expanded in terms of Pauli matrices

$$h' = \vec{r}' \cdot \vec{\sigma} \quad \overrightarrow{r} = (x', y', z')$$

Then from the property (3) we get

$$\det h' = \det h \quad \Rightarrow \quad x'^2 + y'^2 + z'^2 = x^2 + y^2 + z^2$$

Thus relation between $\overrightarrow{r}$ and $\overrightarrow{r}'$ is a rotation. This means that an arbitrary 2×2 unitary matrix U induces a rotation in R_3. This provides a connection between $SU(2)$ and $O(3)$ groups. Note that U and $(-U)$ will give the same rotation.

Example 1 U is diagonal
Then U is of the form,

$$U = \begin{pmatrix} e^{i\alpha/2} & 0 \\ 0 & e^{-i\alpha/2} \end{pmatrix}$$

The 2×2 hermitian matrix h' is

$$h' = UhU^{\dagger} = \begin{pmatrix} e^{i\alpha/2} & 0 \\ 0 & e^{-i\alpha/2} \end{pmatrix} \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix} \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix}$$
$$= \begin{pmatrix} z & (x - iy)\, e^{i\alpha} \\ (x + iy)\, e^{-i\alpha} & -z \end{pmatrix} = \begin{pmatrix} z' & x' - iy' \\ x' + iy' & -z' \end{pmatrix}$$

The relation between new coefficients x', y', z' and the old ones x, y, z are

$$x' = \cos\alpha x + \sin\alpha y$$

$$y' = -\sin\alpha x + \cos\alpha y$$

$$z' = z,$$

This is clearly a rotation of angle α about z-axis.

Example 2 U is real
We can write this as

$$U = \begin{pmatrix} \cos\beta/2 & -\sin\beta/2 \\ \sin\beta/2 & \cos\beta/2 \end{pmatrix}$$

Then the transformation is of the form

$$h' = UhU^{\dagger} = \begin{pmatrix} \cos\beta/2 & -\sin\beta/2 \\ \sin\beta/2 & \cos\beta/2 \end{pmatrix} \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix} \begin{pmatrix} \cos\beta/2 & \sin\beta/2 \\ -\sin\beta/2 & \cos\beta/2 \end{pmatrix}$$
$$= \begin{pmatrix} z\cos\beta - x\sin\beta & x\cos\beta - iy + z\sin\beta \\ iy + x\cos\beta + z\sin\beta & x\sin\beta - z\cos\beta \end{pmatrix} = \begin{pmatrix} z' & x' - iy' \\ x' + iy' & -z' \end{pmatrix}$$

The relations are

$$x' = x\cos\beta + z\sin\beta$$

$$y' = y$$

$$z' = -x\sin\beta + z\cos\beta$$

This is a rotation of angle β about the y-axis.

Rotation group & QM

We now discuss the usage of group theory to study the problems with rotational symmetry in quantum mechanics.
Rotation in R_3 can be represented as linear transformations on the coordinates

$$\vec{r} = (x, y, z) = (r_1, r_2, r_3) \quad , \quad r_i \rightarrow r_i' = R_{ij} X_j \qquad RR^T = 1 = R^T R$$

Consider an arbitary function of coordinates, $f(\vec{r}) = f(x, y, z)$. Under the rotation, the change in f is

$$f(r_i) \rightarrow \; f(R_{ij} r_j) = f'(r_i)$$

If $f = f'$ we say f is invariant under rotation, e.g. $f(r_i) = f(r), r = \sqrt{x^2 + y^2 + z^2}$
In quantum mechanics, we implement the rotation of the coordinates by a unitary operator U operating on the physical states $|\psi\rangle$ with the properties,

$$|\psi\rangle \rightarrow |\psi'\rangle = U|\psi\rangle, \quad O \rightarrow O' = UOU^\dagger$$

so that

$$\Rightarrow \langle\psi'|O'|\psi'\rangle = \langle\psi|O|\psi\rangle$$

This simply means that physical quantites $\langle\psi|O|\psi\rangle$ are independent of the orientation of the coordinate axis.
If $O' = O$, we say O is invariant under rotation,

$$O = UOU^\dagger, \qquad \text{or} \quad UO = OU, \quad \Longrightarrow \qquad [O, U] = 0$$

So rotational invariance of operator O, means it commutes with the roational operator U. In terms of infinitesimal generators of rotation $\overrightarrow{L}$, we have

$$U = e^{-i\theta\vec{n}\cdot\overrightarrow{L}}$$

This implies

$$[L_i, O] = 0, \ \ i = 1, 2, 3$$

For the case where O is the Hamiltonian H, this gives

$$[L_i, H] = 0$$

Let $|\psi\rangle$ be an eigenstate of H with eigenvaule E,

$$H|\psi\rangle = E|\psi\rangle$$

then rotational invariance of H implies

$$(L_i H - HL_i)|\psi\rangle = 0 \quad \Rightarrow \quad H(L_i|\psi\rangle) = E(L_i|\psi\rangle)$$

$i.e$ $\quad |\psi\rangle$ & $l_i|\psi\rangle$ are degenerate. For example, let $|\psi\rangle = |j, m\rangle$ the eigenstates of angular momentum, then $L_{\pm}|j.m\rangle$ are also eigenstates if $|\psi\rangle$ is eigenstate of H. This means for a given l , the degeneracy is $(2l+1)$ as a result of rotional invariance of the Hamiltonian. Take for example the Hamiltonian of the hydrogen atom,

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

which is invariant under the rotation, i.e.

$$[L_i, H] = 0$$

Then the $l = 0$ (s state) is non-degenerate, $l = 1$ (p states) has $2l + 1 = 3$ degeneracy, $l = 2$ (d states) has $2l + 1 = 5$ degeneracy, $\cdots$ *etc*. Thus there is an intimate relation between the dimensionality of irrep and the degeneracy of the eigenstates of the Hamiltonian. Roughly speaking, Hamiltonian can not distinguish between different states within the irrep becasuse of the symmetry.