# Advanced Quantum Mechanics

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Lecture #4

Symmetries and Quantum Mechanics

# Recap of Last Class

- Vibrational Modes of NH3 : Classification of normal modes by symmetry, degeneracies
- The QM Problem: six Harmonic oscillators: classification of states
- Direct Product Representations and their reduction: classification of QM eigenstates
- Irreducible Set of operators and Matrix Elements: Example with 1D SHO

# Matrix Elements: Some Applications

**Vibration modes of $NH_3$:** This is 3D problem, need to think about polarization of light

For plane polarized light, we are interested in matrix element of $\varepsilon . r$

Dipole operator is a vector, find its transformations under the group

Reduce the representation to see what irreps occur in it.

If you are starting from ground state, you can excite modes which transform according to these irreps.

| | E | $2C_3$ | $3\sigma_\nu$ |
|---|---|---|---|
| $A_1$ | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | -1 |
| E | 2 | -1 | 0 |
| $\chi_V$ | 3 | 0 | 1 |

$$\chi_V(R_\theta) = 2\cos\theta + 1 \qquad \chi_V(S_\theta) = 2\cos\theta - 1 \qquad \chi_V(E) = 3$$

So $\chi_V = A_1 \oplus E$

Now $\chi_{vib} = 2A_1 \oplus 2E$

So we have 2 $A_1$ modes and 2 E doublets. All the fundamental modes
are thus excited by radiation.

In fact in this case all modes can be excited by radiation

# Continuous Symmetry and Lie Groups

Symmetry transformations are parametrized by one or more continuous variable

$$G_a \to G(a^{(1)}, a^{(2)}, \ldots a^{(n)}) = G(\vec{a})$$

Group Multiplication for continuous groups

$$G_a G_b = G_c \to G(\vec{a})G(\vec{b}) = G(\vec{c}) \qquad c^{(i)} = F_i[\vec{a}, \vec{b}]$$

These functions essentially serve the purpose of a group table for these groups.

If the n functions $F_i$ are analytic functions

the group is called a n parameter Lie Group

Group Properties:

Associativity:

$$G_a(G_b G_c) = (G_a G_b)G_c$$

$$F[\vec{a}, F[\vec{b}, \vec{c}]] = F[F[\vec{a}, \vec{b}], \vec{c}]$$

Identity:

$$F[0, \vec{a}] = F[\vec{a}, 0] = \vec{a} \qquad E = G(0)$$

Inverse:

$$F[\vec{a'}, \vec{a}] = F[\vec{a}, \vec{a'}] = 0$$

# Examples

Scale Transformation: $x' = e^b x$ Parametrized by 1 real non zero number b

$$x" = e^a x' = e^{a+b} x \qquad c = a + b$$ is the group multiplication rule

Identity is parametrized by 0 and inverse of transf. by b is the scaling by -b

This is a 1 parameter Abelian Lie group

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Translation: $x' = x + a$ Parametrized by 1 real number a

$$x'' = x' + b = x + a + b \qquad c = a + b$$ is the group multiplication rule

Identity is parametrized by 0 and inverse of translation by a is the translation by -a

This is a 1 parameter Abelian Lie group

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Translation + Scale Transformation

$x' = e^{b_1} x + a_1$ Parametrized by 2 real numbers ($a_1$, $b_1$)

$$x'' = e^{b_2} x' + a_2 = e^{b_1+b_2} x + e^{b_2} a_1 + a_2$$

Group multiplication rule:

$$b = b_1 + b_2 \qquad a = e^{b_2} a_1 + a_2$$

Identity is parametrized by (0,0)

Inverse of (a,b) is (-$e^{-b}$a, - b)

This is a 2 parameter Non-Abelian Lie group

# Examples

2D Rotation: $\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$

Group multiplication rule:

$$\theta = \theta_1 + \theta_2$$

U(1): $z = x + iy, \quad z' = x' + iy' \quad z' = ze^{-i\theta}$

1 parameter
Abelian Lie group

Identity is parametrized by $\theta$=0 and inverse of rotation by $\theta$ is rotation by $-\theta$

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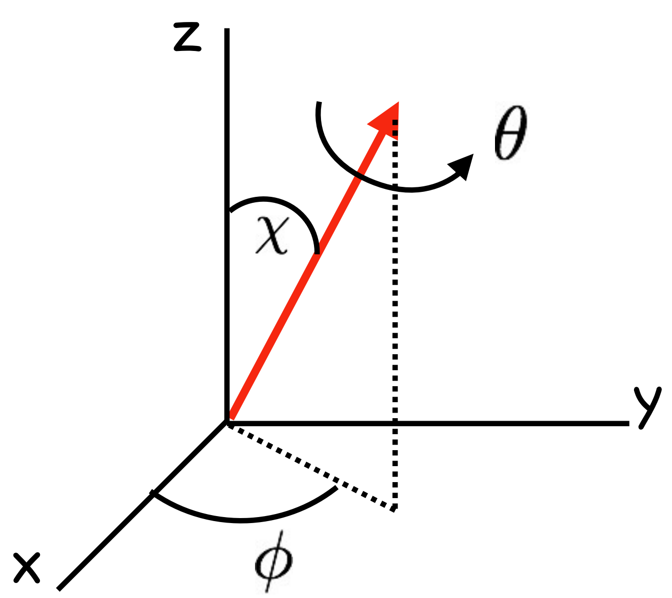
3D Rotation:

3 ways of parametrizing rotations:

1) Axis, angle $\hat{n} = (\chi, \phi), \quad \theta$




Rodrigues Formula:

$$\vec{r}' = \vec{r}\cos\theta + (\hat{n} \times \vec{r})\sin\theta + \hat{n}(\hat{n} \cdot \vec{r})(1 - \cos\theta)$$

For small $\theta$, to linear order in $\theta$, Cos$\theta$ -> 1, Sin$\theta$ —> $\theta$

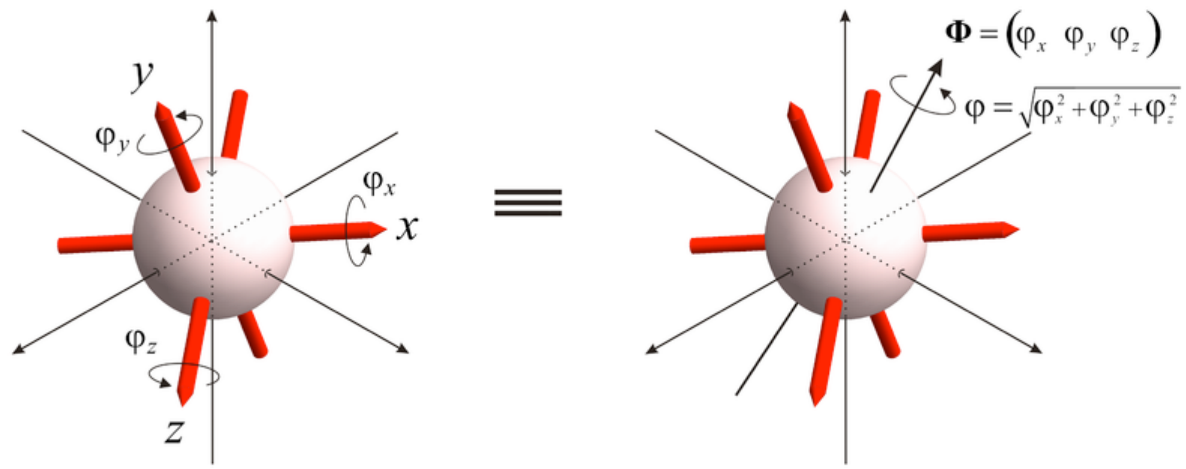
$$\vec{r'} = \vec{r} + (\hat{n} \times \vec{r})\theta$$

# Examples

3 ways of parametrizing rotations:

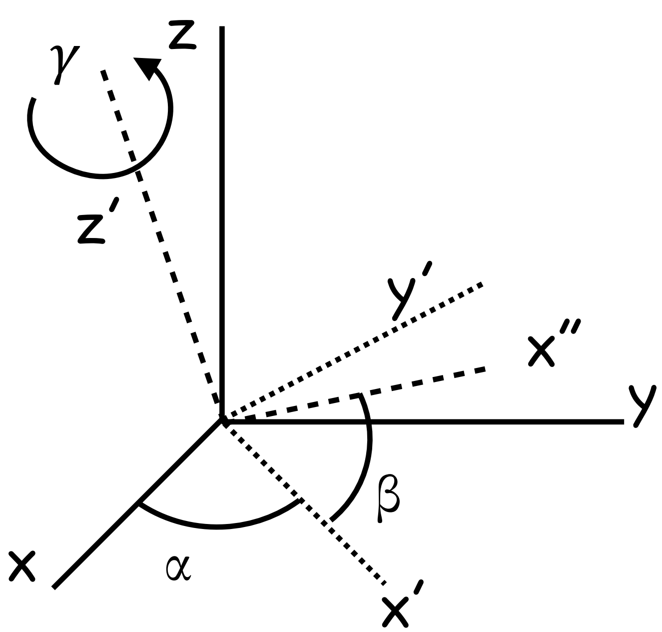
## 3D Rotation:

2) Simultaneous Orthogonal Rotn.




3) Euler angles

$$R_{z'}(\gamma)R_{y'}(\beta)R_z(\alpha)$$




First 2 rotations rotate the z axis to the actual axis of rotation

The last rotation is the actual rotation about this axis

Let the axis of rotation lie in the x′-z plane

$R_z(\alpha)$: Rotn. about z axis, brings x –> x′

$R_{y'}(\beta)$: Rotn. about y′ axis (in x′-z plane) brings z to rotn. axis

$R_{z'}(\gamma)$: Rotn. about z′ axis (actual rotn. axis) by $\gamma$

$$\hat{n} = (\beta, \alpha) \quad \theta = \gamma$$

# Examples

N dim. real vector $(x_1, x_2, \ldots x_N)$

**N Dim Rotation:**

Consider the set of linear transformations on $x_i$, $x'_i = R_{ij}\, x_j$, which preserves the norm $r^2 = x_i x_i$

$$x'_i x'_i = R_{ik} R_{ij} x_k x_j = R^T_{ki} R_{ij} x_k x_j = (R^T R)_{kj} x_k x_j = x_i x_i$$

$R^T R = 1$ ⟶ Set of N dim orthogonal matrices ⟶ O(N)

$R^T R = 1$ ⟶ $\text{Det}(R^T)\,\text{Det}(R) = 1$ ⟶ $\text{Det}(R) = \pm 1$

Matrices with Det( R) = - 1 cannot be smoothly connected to the identity matrix. Consider the set with Det( R) = 1 ⟶ group SO(N). This is the group of rotations in N dim.

SO(N) Matrices can be written as exp(M), where M is a real antisymmetric matrix

Can be parametrized by N(N-1)/2 parameters, corresponding to the indep. parameters of generic N dim antisymmetric matrix.

Examples:

$$M = \begin{pmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{pmatrix} \qquad M = \begin{pmatrix} 0 & a & b & c \\ -a & 0 & d & e \\ -b & -d & 0 & f \\ -c & -e & -f & 0 \end{pmatrix}$$

# Examples

SU(N)

Arbitrary Unitary Matrix $\hat{U} = e^{i\hat{H}}$ , where H is a complex Hermitian matrix ($N^2$ real numbers).

For SU(N), Det[U]=1, which means H is traceless. Hence $N^2$-1 matrix elements

$N^2$-1 parameter Non-Abelian Lie Group

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SU(2)

## Cayley-Klein Parameters

$$U = \begin{pmatrix} z_1 & z_2 \\ -z_2^* & z_1^* \end{pmatrix}$$

$$|z_1|^2 + |z_2|^2 = 1$$

## Pauli Matrices

Arbitrary Traceless 2 X 2 matrix

$$a_x\sigma_x + a_y\sigma_y + a_z\sigma_z = \vec{a}.\vec{\sigma}$$

$$U = e^{i\vec{a}\cdot\vec{\sigma}} = cos(a) + i\vec{\sigma}\cdot\hat{a}\sin(a)$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0^* \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

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

U(2)

$$U = e^{i\gamma}\begin{pmatrix} z_1 & z_2 \\ -z_2^* & z_1^* \end{pmatrix}$$

# Representation of Lie Groups

**Infinitesimal Transformations:**

The basic idea which makes study of Lie group representations is that one needs to study only the properties of infinitesimal transformations characterized by parameters infinitesimally close to 0 ( identity transformation). The properties of the whole group can be deduced from the properties of these infinitesimal transformations.

$$T(\vec{a}) = T(0) + i(-i)\sum_m \frac{\partial T(\vec{a})}{\partial a_m}\Big|_{\vec{a}=0} a_m + \mathcal{O}(a_m^2) \quad = 1 - i\sum_m \hat{J}_m a_m + \mathcal{O}(a_m^2)$$

where $\hat{J}_m = i\frac{\partial T(\vec{a})}{\partial a_m}\Big|_{\vec{a}=0}$ are called infinitesimal operators/generators of the representation.

Criterion for Symmetry $\quad [H, T(\vec{a})] = 0 \rightarrow [H, J_m] = 0 \quad$ for all m

- If T is a unitary representation, then the generators are Hermitian and can possibly represent observables.
- In this case, the generators correspond to conserved quantities and provide the quantum numbers of eigenstates

$$T(\vec{a})T^\dagger(\vec{a}) \simeq (1 - i\hat{J}_m a_m)(1 + i\hat{J}_m^\dagger a_m) \simeq [1 - i a_m(\hat{J}_m - \hat{J}_m^\dagger)] = 1$$

$$\Rightarrow \hat{J}_m = \hat{J}_m^\dagger$$

# Generators of Lie Groups: Examples

**Example:** Translation Invariance $T(\vec{R})\vec{r} = \vec{r} + \vec{R}$

**Infinitesimal Transformation:** $T(\vec{R})\psi(\vec{r}) = \psi(\vec{r} - \vec{R}) \simeq \left[1 - i\vec{R}\cdot\frac{\vec{\nabla}}{i}\right]\psi(\vec{r})$

Corresponding generator is momentum, $\vec{p} = \frac{\vec{\nabla}}{i}$ which is conserved in translation invariant systems

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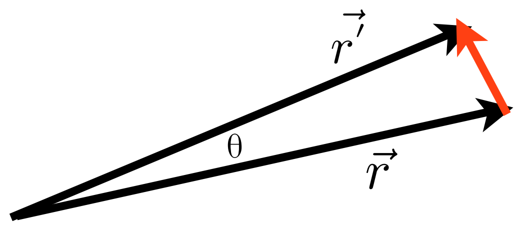
**Example:** Rotational Invariance




Rodrigues Formula for infinitesimal transf.: $\vec{r}' = \vec{r} + (\hat{n}\times\vec{r})\theta$

$$T(\hat{n},\theta)\psi(\vec{r}) = \psi(\vec{r}') \simeq \left[1 - i\theta(\hat{n}\times\vec{r})\cdot\frac{\vec{\nabla}}{i}\right]\psi(\vec{r}) = \left[1 - i\theta\hat{n}\cdot\left(\vec{r}\times\frac{\vec{\nabla}}{i}\right)\right]\psi(\vec{r})$$

$$= \left[1 - i\theta\hat{n}\cdot\vec{L}\right]\psi(\vec{r}) \qquad \vec{L} = \vec{r}\times\vec{p}$$

is the orbital angular momentum.

The operator corresponding to the generator of translation along a direction is the linear momentum operator along that direction and that corresponding to generator of rotations about an axis is the angular momentum operator along that axis.

We will soon see that this is a broader definition.

# Generators of Lie Groups: Examples

Example: N Dim Rotation

$$R = e^{M} = e^{-i(iM)} = e^{-iL} \qquad L = iM \qquad M_{ij} = -M_{ji}$$

For Infinitesimal Transformation, Matrix elements of M are infinitesimal

$$R = 1 - iL = 1 - iL^{ij}\theta^{ij} \qquad L^{ij}_{\mu\nu} = i[\delta i\mu\delta j\nu - \delta i\nu\delta j\mu]$$

Example:

$$L^{12} = i\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} L^{13} = i\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad L^{14} = i\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$L^{23} = i\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad L^{24} = i\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad L^{34} = i\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

# Finite Transformations

How do we generate the representations for the finite transformations from those for infinitesimal transforms?

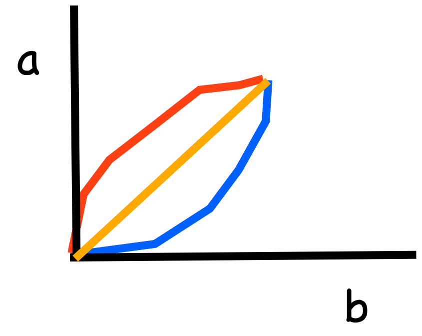
Short Answer: $$T(\vec{a}) = 1 - i\sum_m \hat{J}_m a_m \to T(\vec{a}) = e^{-i\sum_m \hat{J}_m a_m}$$

Consider a one-parameter group. The finite transformation corresponding to the finite parameter a is

$$T(a) = \prod_{i=1}^{n} T_i(a/n) = [T(a/n)]^n$$

For large n --> ∞, a/n is infinitesimal $$T(a) = [1 - i\hat{J}(a/n)]^n \to e^{-i\hat{J}a} \quad \text{as} \quad n \to \infty$$

For a 2 parameter Abelian group with rep. T(a,b)




The final transformation we reach is independent of the path we use as the group is Abelian

So let us choose the diagonal path and break it up into n equal segments

$$T(a) = [1 - i(\hat{J}_a a + \hat{J}_b b)/n]^n \to e^{-i\hat{J}_a a + \hat{J}_b b} \quad \text{as} \quad n \to \infty$$

The form is true for Non-Abelian Groups as well

# Finite Transformations: Examples

Translation Invariance

Infinitesimal Transformation:

$$T(\vec{R})\psi(\vec{r}) = \psi(\vec{r} - \vec{R}) \simeq \left[1 - i\vec{R} \cdot \frac{\vec{\nabla}}{i}\right] \psi(\vec{r})$$

$$= [1 - i\vec{R} \cdot \vec{p}]\psi(\vec{r})$$

Finite Transformation: $T(\vec{R}) = e^{-i\vec{R}.\vec{p}}$

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Rotational Invariance

Axis Angle Formalism

Infinitesimal Transformation:

$$T(\hat{n},\theta)\psi(\vec{r}) = \psi(\vec{r}^{\,'}) \simeq \left[1 - i\theta(\hat{n} \times \vec{r}) \cdot \frac{\vec{\nabla}}{i}\right] \psi(\vec{r}) = \left[1 - i\theta\hat{n} \cdot \left(\vec{r} \times \frac{\vec{\nabla}}{i}\right)\right] \psi(\vec{r})$$

$$= \left[1 - i\theta\hat{n} \cdot \vec{L}\right] \psi(\vec{r})$$

Finite Transformation:

$$\mathcal{D}(\hat{n},\theta) = e^{-i\vec{L}\cdot\hat{n}\theta}$$

$$= e^{-i(\hat{L}_x n_x \theta + \hat{L}_y n_y \theta + \hat{L}_z n_z \theta)}$$

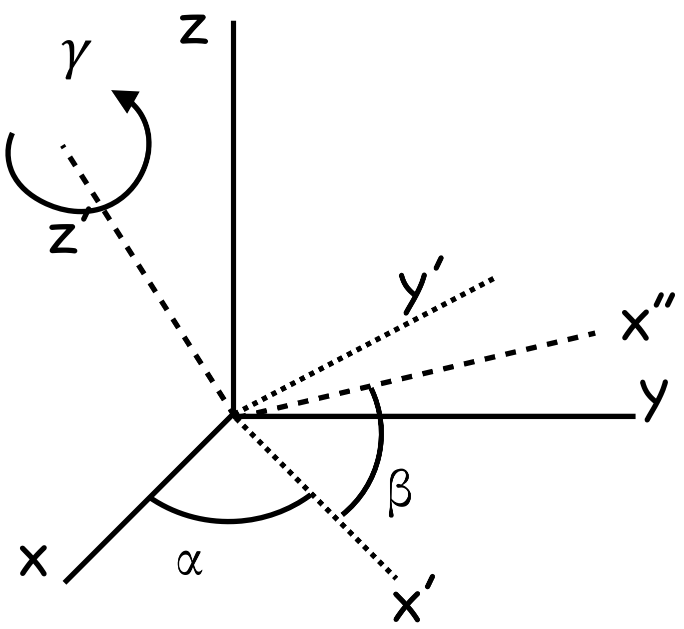
$$= e^{-i(\hat{L}_x \theta_x + \hat{L}_y \theta_y + \hat{L}_z \theta_z)} \qquad \theta_\alpha = \theta n_\alpha$$

Simultaneous rotation about orthogonal axes

# Finite Transformations: Examples

Rotational Invariance

Euler Angle Formalism $R_{z'}(\gamma)R_{y'}(\beta)R_z(\alpha)$




$R_z(\alpha)$: Rotn. about z axis, brings x –> x'

$R_{y'}(\beta)$: Rotn. about y' axis (in x'-z plane) brings z to rotn. axis

$R_{z'}(\gamma)$: Rotn. about z' axis (actual rotn. axis) by $\gamma$

$$R_{z'}(\gamma)R_{y'}(\beta)R_z(\alpha) = R_{y'}(\beta)R_z(\gamma)R_{y'}^{-1}(\beta)R_{y'}(\beta)R_z(\alpha)$$

$$= R_{y'}(\beta)R_z(\gamma)R_z(\alpha)$$

$$= R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha)R_z(\gamma)R_z(\alpha)$$

$$= R_z(\alpha)R_y(\beta)R_z(\gamma)$$

Note the reversal of order

Rotations about fixed axes

Finite Rotation Operator:

$$\mathcal{D}(\alpha,\beta,\gamma) = \mathcal{D}_z(\alpha)\mathcal{D}_y(\beta)\mathcal{D}_z(\gamma) = e^{-iL_z\alpha}e^{-iL_y\beta}e^{-iL_z\gamma}$$

From now on, focus on the generators and their properties

# Generators and Lie Algebra

Parametrization of a Continuous Group is not unique

E.g. For translation group, any orthogonal co-ordinate system could be chosen (x-y-z is arbitrary).
The translation vectors form a 3D real vector space and any orthogonal basis would suffice.

E.g. For rotation group, simultaneous rotation about any orthogonal axes could be chosen.
$(\theta_x,\theta_y,\theta_z)$ form a 3D real vector space and any orthogonal basis would suffice.

Corresponding to a choice of basis in this 3D real vector space, we have a particular realization of generators.

So the generators themselves form a basis in 3D real vector space.

On top of this,

For any representation of a Lie group, the infinitesimal operators satisfy

$$[\hat{J}_m, \hat{J}_n] = \sum_p c^p_{mn} \hat{J}_p$$

$c^p_{mn}$ → Property of the group
Same for all representations

Structure Constants

Lie Bracket

The space of generators, together with the Lie Bracket, is called the Lie Algebra of the group

# Lie Bracket

Not Identity for Non-Abelian Groups

Consider $T(\vec{a})T(\vec{b})T^{-1}(\vec{a})T^{-1}(\vec{b}) = T(\vec{c}) = 1 - i\sum_k c_k \hat{J}_k$

$$= \left[1 - i\sum_m a_m \hat{J}_m - \frac{1}{2}\sum_{mn} a_m a_n \hat{J}_m \hat{J}_n\right]\left[1 - i\sum_p b_p \hat{J}_p - \frac{1}{2}\sum_{pq} b_p b_q \hat{J}_p \hat{J}_q\right]\left[1 + i\sum_m a_m \hat{J}_m - \frac{1}{2}\sum_{mn} a_m a_n \hat{J}_m \hat{J}_n\right]\left[1 + i\sum_p b_p \hat{J}_p - \frac{1}{2}\sum_{pq} b_p b_q \hat{J}_p \hat{J}_q\right]$$

Linear Terms vanish

$$= 1 - \sum_{mp} a_m b_p \hat{J}_m \hat{J}_p + \sum_{mn} a_m a_n \hat{J}_m \hat{J}_n + \sum_{mp} a_m b_p \hat{J}_m \hat{J}_p + \sum_{mp} a_m b_p \hat{J}_p \hat{J}_m + \sum_{pq} b_p b_q \hat{J}_p \hat{J}_q - \sum_{mp} a_m b_p \hat{J}_m \hat{J}_p$$
$$- \sum_{mn} a_m a_n \hat{J}_m \hat{J}_n - \sum_{pq} b_p b_q \hat{J}_p \hat{J}_q$$

$$= 1 - \sum_{mp} a_m b_p [\hat{J}_m, \hat{J}_p]$$

c ~ ab and $[J_m , J_p]$ must be a linear combination of generators.

Further, this depends on group combination rules, and not on particular representations

So $$[\hat{J}_m, \hat{J}_n] = \sum_p c^p_{mn} \hat{J}_p$$

Structure const. are property of group, not of any particular representation.