# Lecture synopsis

## *NTMF061: Group theory and its application in physics*

Winter term 2022/23

### Literature:

Problems are taken mostly from

- Ma, Z.-Qi: Group Theory for Physicists (World Scientific, 2007)
- Inui, Tanabe, Onodera: Group Theory and Its Applications in Physics (Springer, 1996)

### Week 1: October $5^{th}$

- **group definition, order of the group**, examples of groups, Abelian group
- multiplication table, **rearrangement theorem:** *Each row and each column of the multiplication table contains each element of the group once and only once.*
- **subgroup**, order of an element, cyclic subgroup, **theorem:** *Intersection of two subgouprs of $G$ is again a subgroup of $G$.*
- **left and right cosets with respect to a subgroup**, *each element of $G$ is a member of one and only one left/right coset with respect to a given subgroup*
- **Lagrange theorem:** *Order of a subgroup of $G$ divides $\#G$*, index of a subgroup
- **conjugacy classes**, **theorem:** *Number of elements in any class $(g)$ is a divisor of $\#G$.*

*Tutorial:* Classification of point groups, symmetry elements, and symmetry operations

### Suggested problems:

- Let $g$ and $h$ be elements of order two. Show that if $g$ and $h$ commute, the set $V_4 = \langle g, h\rangle = \{e, g, h, g \cdot h\}$ constitutes a group (called four-group). Construct its multiplication table. Are there other groups of order 4?
- Demonstrate that the set of rotations through 180° around the $x-$, $y-$ and $z-$axes and the identity transformation, $D_2 = \{E, C_{2x}, C_{2y}, C_{2z}\}$, constitutes a group and its multiplication table is that of a four-group $V_4$.
- Verify that if two mirror planes $\sigma_1$ and $\sigma_2$ form an angle $\theta$, the product operation $\sigma_1\sigma_2$ is the rotation $R(2\theta)$ whose rotation axis is the intersection of the two mirror planes.
- Find the eight proper subgroups of $C_{4v}$.
- Derive the left and right coset decomposition of $C_{3v}$ with respect to its proper subgroups.
- Prove that elements belonging to the same class have the same order.

## Week 2: October $12^{th}$

- multiplication of conjugacy classes, **class constants** $(g_i)(g_j) = \sum_{(g_k)} c_{ij}^k (g_k)$
- **normal (invariant) subgroup**, center of a group, simple and semi-simple groups
- **theorem:** $H \triangleleft G \Leftrightarrow H$ *consists entirely of complete classes of* $G$.
- product of left/right cosets, **theorem (factor group):** *The set of all distinct cosets with respect to an invariant subgroup* $H \triangleleft G$ *forms a factor (quotient) group.*
- **homomoprhic mapping**; surjective, injective and bijective (**isomorphic**) mappings
- **theorem:** *Let* $\Phi : G \to G'$ *be a homomorphism. Then* $\mathrm{Im}\, \phi$ *is a subgroup of* $G'$, $\mathrm{Ker}\, \phi$ *is invariant subgroup of* $G$ *and* $Im\, \phi \sim G/\mathrm{Ker}\, \phi$.
- **direct and semi-direct product groups**, Euler group as a semi-direct group

### Suggested problems:

- Construct the class multiplication table for $C_{4v}$.
- The inverse elements of $n_j$ elements constituting class $(g_j)$ form a class by themselves, which will be denoted $(g_{j'})$. Show that $c_{ij}^1 = n_i$ when $(g_i) = (g_{j'})$ and $c_{ij}^1 = 0$ otherwise $[(g_1) = e]$.
- Show that $(g_i)(g_j) = (g_j)(g_i)$.
- show that the conjugation $\phi_a : g \mapsto aga^{-1}$ is an isomorphism
- show that left translation $L_a : g \mapsto ag$ is an isomorphic mapping but that it is not homomorphic
- show that the group $D_{3h} \sim C_{3v} \otimes C_s \sim D_3 \otimes C_s$
- For the point group $C_{6v}$
  - construct the multiplication table
  - find the set of generators
  - find the six classes
  - explain why the rotations fall into two distinct classes
  - construct the multiplication table of the classes (class constants)
  - find the four proper invariant subgroups
  - find the corresponding coset decompositions
- Show that up to isomorphism, there are only two different fourth-order groups – the cyclic group and the four-group $V_4$.

- Show that a group must be abelian if the order of any element in the group, except for the identity, is 2.
- In a finite group $G$ of order $\#G$, let $(g) = \{g_1, \ldots, g_n\}$ be a class containing $n$ elements. For any two elements $g_i$ and $g_j$ in the class (may be different or same), show that the number $m$ of elements $h \in G$ satisfying $g_i = hg_jh^{-1}$ is $m = \#G/n$.

## Week 3: October $19^{th}$

- **group action on a set**, orbit, stabilizer (isotropy) group, **theorem:** *Let $G$ be a finite group acting on a set $\mathcal{M}$. Then $(\#G \cdot m)(\#G_m) = \#G$.*
- Group action on itself: left/right translation, conjugation
- **representation of a group as an action on a vector space** (homomorphism to the group of all automorphisms on the vector space), dimension of the representation, faithful representation
- basis of a representation, **matrix representation**
- **equivalent representations**, intertwining mapping; equivalent matrix representations are related by similarity transformation
- invariant subspaces under group action, **reducible and irreducible representation**, subrepresentation, reducibility of matrix representations
- **completely reducible representation**, block-diagonal form of completely reducible matrix representation
- **theorem:** *Every irreducible representation of a finite group is finite-dimensional.*
- **unitary representation**, **theorem:** *Every finite-dimensional reducible unitary representation of a group $G$ is completely reducible.*
- **theorem:** *Every finite-dimensional representation of a finite or compact Lie group is equivalent to some unitary representation.*
- **theorem (Maschke):** *Every finite-dimensional reducible representation of a finite or compact Lie group is completely reducible.*
- **Schur lemma I:** *Intertwining mapping between two irreducible representations is either bijective (and the two representations are equivalent) or null mapping.*
- **Schur lemma II:** *Let $(\rho, V)$ be a complex finite-dimensional irreducible representation of a group $G$ and $S$ an intertwining operator on $V$ commuting with all operators $T(g) \in \rho$. Then $S = \lambda \mathbb{1}$ for $\lambda \in \mathbb{C}$.*
- **theorem:** *Complex finite-dimensional irreducible representations of an Abelian group are one-dimensional.*

**Suggested problems:**

- Let $G$ be a non-Abelian group, $D(G)$ its faithful representation, and $D(g)$ the matrix representing an element $g \in G$. Assuming we replace the set of matrices $D(g)$ by another set as indicated below, decide whether the new set still forms a representation:

  1. $g \mapsto D(g)^\dagger$
  2. $g \mapsto D(g)^T$
  3. $g \mapsto D(g^{-1})$
  4. $g \mapsto D(g)^*$
  5. $g \mapsto D(g^{-1})^\dagger$
  6. $g \mapsto \det D(g)$
  7. $g \mapsto \mathrm{Tr}\, D(g)$

- Prove that the module of any representation matrix in a one-dimensional representation of a finite group is equal to 1.

## Week 4: October 26$^{th}$

- **theorem:** *Orthogonality relations for irreducible matrix representations*

$$\sum_{g\in G}[D^\mu(g^{-1})^i_j]D^\nu(g)^k_l = \frac{\#G}{d_\mu}\delta_{\mu\nu}\delta_{jk}\delta_{il}$$

$$\text{for unitary repre:}\ \sum_{g\in G}[D^\mu(g)^j_i]^*D^\nu(g)^k_l = \frac{\#G}{d_\mu}\delta_{\mu\nu}\delta_{jk}\delta_{il}$$

- **character of a representation**

- **theorem:** *Orthogonality relations for characters*

$$\sum_{g\in G}\chi^\mu(g)^*\chi^\nu(g) = \#G\delta_{\mu\nu}$$

- **theorem:** *For finite or compact Lie group, equality of characters of two representations is a sufficient condition for their equivalence.*

- decomposition of a reducible representation $\rho$ (of a finite or compact Lie group):

$$\rho = \oplus_\mu n_\mu \rho^\mu \Longrightarrow n_\mu = \frac{1}{\#G}\sum_g \chi^\mu(g)^*\chi(g)$$

  with summation running over all non-equivalent IRREPs $\rho^\mu$.

- regular representation of a finite group, **theorem:** $\#G = \sum_\mu d_\mu^2$
- **theorem:** *Number of non-equivalent IRREPs of a finite group is equal to the number of distinct conjugacy classes.*
- **theorem (Frobenius):** *Representation* $(\rho, V)$ *of a finite group* $G$ *is irreducible*

$$\iff \sum_{(g_k)} n_k \chi(g_k)^* \chi(g_k) = \#G.$$

*Tutorial:*

1. Vector and pseudo-vector representation of $O(3)$

**Suggested problems:**

- Consider $C_{3v}$ point group.
  1. Verify that the second Schur lemma holds for the irreducible representation $E$.
  2. Show that for the "defining" 3-dim representation (action on $\mathbb{R}^3$) there exists a matrix other than $\mathbb{1}$ that commutes with all matrices of the representation.
- Prove that the similarity transformation matrix between two equivalent irreducible unitary representations of a finite group, if restricting its determinant to be equal to one, has to be unitary.
- Show that for a finite group $G$, the sum of the characters of all elements in any irreducible representation of $G$, except for the trivial representation, is equal to zero.

## Week 5: November $2^{th}$

- transformation of a wave function [group action on a Hilbert space $\mathcal{L}^2(\mathbb{R}^3)$]; transformation of an operator
- **direct product representation**, symmetric and antisymmetric products of equivalent representations
  - point groups – transformation of quadratic (or higher polynomial) functions
- **symmetrization (projection) operators** (complete and incomplete), construction of a basis of irreducible (sub)representation

*Tutorial:*

1. Character table for $D_{3h}$
2. MO-LCAO for $H_3^+$ – basis symmetrization

**Suggested problems:**

- If the group $G$ is a direct product $H_1 \otimes H_2$ of two subgroups show that the direct product of two irreducible representations of two subgroups is an irreducible representation of $G$.

  - Considering the number of classes in $H_1$, $H_2$ and in $G$, show that each irreducible representation of $G$ can be constructed as a direct product representation of irreducible representations of $H_1$ and $H_2$. You also have to show that the direct product of inequivalent pairs of irreducible representations of $H_i$'s gives inequivalent irreducible representations of $G$.

- The homogeneous function space of degree 2 spanned by the basis functions

$$\psi_1(x, y) = x^2, \quad \psi_2(x, y) = xy, \quad \psi_3(x, y) = y^2$$

  is invariant in the rotations $R$,

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = R \begin{pmatrix} x \\ y \end{pmatrix},$$

  1. $R = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
  2. $R = \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}$
  3. $R = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}$.

  Calculate the matrix form $D(R)$ of the corresponding transformation operators $U(R)$ in the three-dimensional function space.

- Consider the point group $D_3$ as a coordinate transformation in $\mathbb{R}^2$ (i.e., its irreducible representation $E$). Find the two generators of the group, $g_1$ and $g_2$, and construct the corresponding $2 \times 2$ matrices $D^E(g_1)$ and $D^E(g_2)$.

  1. Let the four-dimensional function $V_4$ space be spanned by the following basis:

$$\psi_1 = x^3, \quad \psi_2 = x^2 y, \quad \psi_3 = xy^2, \quad \psi_4 = y^3.$$

     Find the corresponding representation matrices of the generators $g_1$ and $g_2$. Decompose this representation into the direct sum of irreducible representations of $D_3$, and transform the basis functions such that the new basis functions transform according to those irreducible representations (i.e., find the respective invariant subspaces of $V_4$).

## Week 7: November $16^{rd}$

- **symmetries in quantum mechanics**
  - symmetry group as a group of transformations leaving Hamiltonian of the system invariant
  $$\tilde{H} = U(g)HU(g)^{\dagger} = H$$
  - eigenfunctions of the Hamiltonian as a basis of an irreducible representation of the symmetry group, degeneration of energy levels (normal and accidental, hidden symmetries)
- matrix elements of **invariant scalar operators**
$$U(g)\Omega U(g)^{\dagger} = \Omega \implies \langle \psi_k^{\mu} | \Omega | \varphi_l^{\nu} \rangle = h^{\mu} \delta_{\mu\nu} \delta_{kl}$$
- decomposition of direct product representation – **Clebsch-Gordan series**
- basis of direct product representation – **Clebsch-Gordan coefficients**
- selection rules for **matrix elements of invariant scalar operators**
- **irreducible tensor operators**, **Wigner-Eckart theorem**
- **molecular vibrations** and optical transitions
  - **normal coordinates** (vibrational modes) as bases of IRREPs of the symmetry group
  - activity of vibrational modes in infrared spectrum and in Raman scattering

*Tutorial*

1. MO-LCAO for $H_3^{2+}$ – the Hamiltonian

### Suggested problems:

- Calculate the unitary similarity transformation matrix $X$ for reducing the self-direct product of the three-dimensional irreducible unitary representation $\rho^T$ of the point group **T**:
$$X^{-1}\left[D^T(g) \otimes D^T(g)\right] X = \bigoplus_{\sigma} n_{\sigma}^{(T\otimes T)} D^{\sigma}(g)$$
- Calculate the Clebsch-Gordan series and the Clebsch-Gordan coefficients in the reduction of the direct product representation $\rho^{T_1} \otimes \rho^{T_2}$ of the point group **I**.
- Examine the selection rules for Raman scattering by a $H_2O$ molecule.

## Week 8: November $23^{th}$

- **Symmetric (permutation) group $\mathcal{S}_n$**
  - composition rule, decomposition into disjoint cycles, composition of cycles
  - classes (elements with the same cycle structure)
  - transpositions
  - even permutations as invariant subgroup, generators of $\mathcal{S}_n$
  - irreducible representations of $\mathcal{S}_n$: Young diagrams, Young tableau, hook rule (dimensions of IRREPs)
  - bases of IRREPs of $\mathcal{S}_n$ – subduction chain $\mathcal{S}_n \downarrow \mathcal{S}_{n-1} \downarrow \cdots \downarrow \mathcal{S}_1$
  - characters of IRREPs of $\mathcal{S}_n$
  - orthogonal matrix representation

*Tutorial:*

1. Character table of $\mathcal{S}_4$

### Suggested problems:

- There are 52 pieces of playing cards in a set of poker. The order of cards is changed in a shuffle according to the following rule: The deck is split into two parts in equal number, then one card is picked from each part in order. The first and the last cards thus do not change their positions, the remaining are rearranged. Find the corresponding permutation, decompose it into a product of disjoint cycles, and determine how many shuffles are needed to take the deck into its original order.
- Find the dimensions of irreducible representations of $\mathcal{S}_7$
- Find explicit form of the two-dimensional irreducible orthogonal matrix representation of $\mathcal{S}_3$.
- Calculate the representation matrices of the generators of $\mathcal{S}_4$ by induction from the representation found in the previous task and reduce them into irreducible representations.
- Implement a code that will generate the character table of an arbitrary permutation group.

## Self-study

- relations between representations of a group and its subgroups
  - **subduced and induced representations**, decomposition to irreducible representations
  - **theorem (Frobenius reciprocity):** $\alpha_{\mu}^{\nu\uparrow G} = \alpha_{\nu}^{\mu\downarrow H}$

*Tutorial*

1. Induced representations, Frobenius reciprocity
2. Optical transitions in $CO_3^{2+}$ ion
3. Normal coordinates for diatomic molecule

### Suggested problems:

- Show that induction from the trivial representation of the trivial subgroup $\{E\}$ gives the regular representation of a group $G$.
- Construct the induced representations of $C_{3v}$ from the $A'$ and $A''$ irreducible representations of $C_s$ and verify Frobenius reciprocity theorem.
- Consider the 5-dimensional representation $l = 2$ of $SO(3)$ with characters given by the general formula

$$\chi^l(C_\varphi) = \frac{\sin[(l+1/2)\varphi]}{\sin(\varphi/2}).$$

  Construct the subduced representations $\rho^{l=2}_{SO(3)\downarrow O}$ and $\rho^{l=2}_{SO(3)\downarrow D_4}$ and find their reduction to irreducible representations of the subgroups $O < SO(3)$ and $D_4 < SO(3)$.
- Show that $\rho^{\mu}_{\uparrow G}$ is irreducible if and only if the irreducible representation $\rho^\mu$ of $H$ appears in $(\rho^{\mu}_{\uparrow G})_{\downarrow H}$ only once.

## Week 9: November 30$^{st}$

**LIE GROUPS**

- $SO(3)$ **as a group of orthogonal matrices** $3 \times 3$ **with unit determinant**
  - **linearization** – antisymmetic matrices as generators of infinitezimal rotations
  - general rotation as **exponential** of the generators
  - group $O(3)$ has the same generators but exponential mapping covers only the connected subgroup $SO(3)$
  - generators of rotations form **Lie algebra** $\mathfrak{so}(3)$ with **structure constants**

$$[J_i, J_j] = ic_{ij}^k J_k, \qquad c_{ij}^k = \varepsilon_{ijk}$$

  - $(J_i)_{jk} = -ic_{ij}^k$ is **adjoing representation** of the Lie algebra $\mathfrak{so}(3)$
- **Review of differential geommetry**
  - **topological space**, open and closed sets, neighborhood of a point, **continuous mapping**, homeomorphism
  - **connected**, **path-connected** and **simply-connected** topological spaces, **compactness**
  - **topological manifold**, **coordinate map**, atlas, **differentiable manifolds** (smooth, analytical)
- **Lie groups as smooth manifolds**
  - **smooth mapping** between manifolds
  - **real Lie group**, linear Lie group
  - global topological properties of Lie groups – $E(2)$, $SO(2)$, $SO(3)$, $SU(2)$, $SL(2, \mathbb{R})$

## Week 10: December 8$^{th}$

**LIE ALGEBRAS – left-invariant vector fields on Lie groups**

- **tangent vectors** as a class of equivalence of tangent curves, tangent space $T_pM$, directional derivative, **isomorphism of** $T_pM$ **and the space of derivatives** $D_pM$, tangent bundle
- **vector field**, **integral curve** of a vect. field
- **push-forward mapping**
- **Lie bracket**

- **left-invariant vector field**, **isomorphism of $T_eG$ and the space** $\mathcal{L}(G)$ of left-invariant fields on a Lie group $G$
- push-forward of Lie bracket, commutator of vectors from $T_eG$ using Lie bracket of the corresponding fields from $\mathcal{L}(G)$, $T_eG$ **as Lie algebra of** $G$

**Exponential mapping**

- **one-parameter subgroup** of a LG
- **theorem:** Every one-parameter subgroup of $G$ is an integral curve of some left-invariant vector field and every integral curve of a left-invariant vector field is one-parameter subgroup.
- **theorem:** Left-invariant vector fields on $G$ are complete.
- **exponential mapping** from LA $\mathcal{G}$ to LG $G$:

$$\exp : \mathcal{G} \to G \quad X \mapsto \exp(X) \equiv \gamma^X(1)$$

  *for* $\gamma^X(t) \subset G$ *the one-parameter subgroup corresponding to* $X \in \mathcal{G}$*.*

- $\gamma^X(t) = \exp(tX)$
- **theorem:** Exponential mapping is a local diffeomorphism between $T_eG$ and $U(e) \subset G$
- connected subgroup, **theorem:** Let $G$ be compact LG, then every element of its connected subgroup can be written as $g = \exp(X)$ for some $X \in \mathcal{G}$.
- **theorem:** Every connected component of a LG is a right coset with respect to the connected subgroup.
- **theorem:** Every point of the connected subgroup of $G$ can be written as a finite product of exponential elements.
- **theorem:** Every connected component of a Lie group is a right coset of its connected subgroup.

*Tutorial:*

1. matrix groups and their algebras (left-invariant fields, structure constants and commutator on $T_eG$) – $\mathfrak{gl}(n, \mathbb{R})$

## Week 11: December $14^{th}$

**Relations between Lie groups and their Lie algebras**

- **homomorphism and isomorphism** between LAs
- derived homomorphism of LAs, LA of a subgroup of $G$ is sub-algebra of the LA of $G$
- **theorem:** "Let $\Phi$ be isomorphism between two LGs. Then the derived homomorphism $\Phi_*$ is an isomorphism between corresponding LAs."
- discrete subgroup, **theorem:** "If the kernel of a surjective homomorphism $\Phi$ between two LGs is discrete, then the derived homomorphism $\Phi_*$ is an isomorphism between corresponding LAs."
- relation between non-isomorphic LGs with isomorphic LAs, **universal covering group**

**Killing-Cartan form – recovering the geometry of LG from LA**

- representation of LA as a homomorphism $\mathcal{G} \to \mathrm{End(V)}$, **adjoint representation**
- **Killing-Cartan form** and metric, properties of K-C form

*Tutorial:*

1. Homomorphism (double covering) $SL(2,\mathbb{C}) \to L_+^\uparrow$ and $SU(2) \to SO(3)$
2. Killing-Cartan form on $\mathfrak{sl}(2,\mathbb{R})$ – compact and non-compact generators