Lecture synopsis

NTMF061: Group theory and its application in physics

Winter term 2021/22

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: September 29^{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 subgroups 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 $V_4 = \langle g, h \rangle = \{e, g, h, g \circ h\}$ constitutes a group (called four-group).
- 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 σ_1 and σ_2 form an angle θ , 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 6^{th}

- multiplication of conjugacy classes, class constants $(g_i)(g_j) = \sum_{(q_k)} c_{ij}^k(g_k)$
- 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.
- homomorphic mapping, kernel and image of a homomorphism
- surjective, injective and bijective (isomorphic) mappings
- theorem: Let $\Phi: G \to G'$ be a homomorphism. Then $\operatorname{Im} \phi$ is a subgroup of G', $\operatorname{Ker} \phi$ is invariant subgroup of G and $\operatorname{Im} \phi \sim G/\operatorname{Ker} \phi$.
- canonical projection of G onto $G/H: g \mapsto gH$
- 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 $c_{ij}^k = n_i$ when $(g_i) = (g_{j'})$ and $c_{ij}^k = 0$ 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} has the structrure of a direct product $C_{3v} \otimes C_{1h}$
- 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 13^{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.

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. $g \mapsto \operatorname{Tr} D(g)$
- Prove that the module of any representation matrix in a one-dimensional representation of a finite group is equal to 1.

Week 4: October 20th

- Schur lemma I: Intertwining mapping between two irreducible representations is either isomorphic (and the two representations are equivalent) or null mapping.
- Schur lemma II: Let (ρ, V) be a complex finite-dimensional irreducible representation of a group G and S an intertwining operator on V commuting with all operators $T(g) \ \forall g \in G$ from the representation. Then $S = \lambda \mathbb{1}$ for $\lambda \in \mathbb{C}$.
- theorem: Complex finite-dimensional irreducible representations of an Abelian group are one-dimensional.
- theorem: Orthogonality relations for irreducible matrix representations

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

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

- 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 sufficient condition for their equivalence.
- decomposition of a reducible representation ρ (of a finite or compact Lie group):

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

with summation running over all non-equivalent IRREPs ρ^{μ} .

- 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 (ρ, V) of a finite group G is irreducible

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

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 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: October 27th

- vector and pseudo-vector representation of O(3)
- character table of D_{3h}
- 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

• transformation of quadratic functions

Tutorial:

- 1. Vector and pseudo-vector representation of O(3)
- 2. Character table for D_{3h}

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 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 give inequivalent irreducible representations of G.
- The homogeneous function space of degree 2 spanned by the basis functions

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

is invariant in the rotations R,

$$\left(\begin{array}{c} x' \\ y' \end{array}\right) = R \left(\begin{array}{c} x \\ y \end{array}\right),$$

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 2×2 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:

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

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 6: November 3^{rd}

- symmetrization (projection) operators (complete and incomplete), construction of a basis of irreducible (sub)representation
- symmetries in quantum mechanics
 - symmetry group as a group of transformations leaving the Hamiltonian of a system invariant

$$\tilde{H} = U(g)HU(g)^{\dagger} = H$$

- eigenfunctions of the Hamiltonian as a basis of irreducible representation of the symmetry group, degeneration of energy levels (normal and accidental, hidden symmetries)
- matrix elements of invariant scalar operators

$$U(g)\Omega U(g)^{\dagger} = \Omega \implies \langle \psi_k^{\mu} | \Omega | \varphi_l^{\nu} \rangle = h^{\mu} \delta_{\mu\nu} \delta_{kl}$$

- 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. MO-LCAO for H_3^{2+} the Hamiltonian
- 2. Induced representations, Frobenius reciprocity (self-study)

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 $\rho_{SO(3)\downarrow O}^{l=2}$ and $\rho_{SO(3)\downarrow D_4}^{l=2}$ and find their reduction to irreducible representations of the subgroups O < SO(3) and $D_4 < SO(3)$.

• Show that $\rho_{\uparrow G}^{\mu}$ is irreducible if and only if the irreducible representation ρ^{μ} of H appears in $(\rho_{\uparrow G}^{\mu})_{\downarrow H}$ only once.

Week 7: November 10^{th}

- 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. Optical transitions in CO_3^{2+} ion
- 2. Normal coordinates for diatomic molecule (self-study)

Suggested problems:

• Calculate the unitary similarity transformation matrix X for reducing the self-direct product of the three-dimensional irreducible unitary representation ρ^T of the point group \mathbf{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**.
- \bullet Examine the selection rules for Raman scattering by a H_2O molecule.

Week 8: November 24th

- Symmetric (permutation) group 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 S_n : Young diagrams, Young tableau, hook rule (dimensions of IRREPs)
 - bases of IRREPs of S_n subduction chain $S_n \downarrow S_{n-1} \downarrow \cdots \downarrow S_1$
 - characters of IRREPs of S_n
 - orthogonal matrix representation

Tutorial:

1. Character table of 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 S_7
- Find explicit form of the two-dimensional irreducible orthogonal matrix representation of S_3 .
- Calculate the representation matrices of the generators of 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.

Week 9: December 1^{st}

LIE GROUPS

- SO(3) as a group of orthogonal matrices 3×3 with unit determinant
 - linearization antisymmetric 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
 - topological group, **smooth mapping**, **real Lie group**, linear group
 - global topological properties of Lie groups E(2), SO(2), SO(3), SU(2)

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
- theorem (Ado): Every finite-dimensional abstract LA is isomorphic to some LA of square matrices with std. commutator.

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 $X \in \mathcal{G}$.

•
$$\gamma^X(t) = \exp(tX)$$

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 15^{th}

Exponential mapping

- 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 $q = \exp(X)$ 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.

Relations between Lie groups and their Lie algebras

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

Tutorial:

1. Homomorphism (double covering) $SL(2,\mathbb{C}) \to L_+^{\uparrow}$ and $SU(2) \to SO(3)$ (for English version, see Sternberg, Sec. 1.2)

Week 12: December 22^{nd}

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

- invariant sub-algebra, simple and semi-simple LA a LG
- representation of LA on V as a homomorphism $\mathcal{G} \to \operatorname{End}(V)$, matrix representation of LA
- adjoint representation of LA
- Killing-Cartan form and metric, properties of K-C form
- solvable LA, theorem: Cartan criteria for solvable and semi-simple LA
- **theorem:** LG *G* is compact if and only if the C-K form on the corresponding LA is negative definite.

Representations of LA

- analytical representation of a LG, **theorem:** "Relations between the analytical representation of LG and the corresponding representation of LA"
- theorem: "Irreducibility of the corresponding representations of LG and LA"
- relations between the representations of SO(3) and $\mathfrak{so}(3) \sim \mathfrak{su}(2)$, multi-valued representations and the universal covering group

Tutorial:

- 1. Killing-Cartan form on $\mathfrak{sl}(2,\mathbb{R})$
- 2. Left-invariant measure on SU(2) and SO(3)

Suggested problems:

• Prove that the elements $u(\omega, \mathbf{n})$ with the same ω form a class in SU(2)

Week 13: January 5^{th}

Complexification of LA

- ullet complexification of a real LA with generators that are linearly dependent over ${\mathbb C}$
- relations of representations of real and complexified LA

Irreducible representations of semi-simple LA

- **theorem:** "semi-simple LA is either simple or isomorphic to a direct sum of its simple ideals"
- **theorem:** "LA of a direct product Lie group is isomorphic to a direct sum of the corresponding Lie algebras"
- Casimir operator, the quadratic Casimir operator for semi-simple LA
- rank LG/LA, Racah theorem
- irreducible representations of $\mathfrak{su}(2)$ and $\mathfrak{so}(1,3) \sim \mathfrak{sl}(2,\mathbb{C})$

$$-\mathfrak{so}(1,3)_{\mathbb{C}}\sim\mathfrak{su}(2)_{\mathbb{C}}\oplus\mathfrak{su}(2)_{\mathbb{C}}$$

- the adjoint representation of LA and LG
- **theorem:** "Adjoint representation of a semisimple LA is faithful, the adjoint representation of a simple LA is irreducible."