

Lie theory and Physics

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Preface

Sophus Lie (1842-1899) was a Norwegian mathematician, who created an *algebraic* language (Lie algebras) to deal with the notion of symmetry in the *analytic* setting (Lie groups).

1 Constructions of linear algebra

Suppose U, V are two finite dimensional complex vector spaces. The set theoretic direct product $U \times V$ has a natural vector space structure by componentwise addition and scalar multiplication, so

$$(u_1, v_1) + (u_2, v_2) := (u_1 + u_2, v_1 + v_2), \quad \lambda(u, v) := (\lambda u, \lambda v)$$

for all $u_1, u_2, u \in U$, $v_1, v_2, v \in V$ and $\lambda \in \mathbb{C}$. This vector space is denoted $U \oplus V$ and is called the *direct sum* of U and V . It is easy to check that $\dim(U \oplus V) = \dim U + \dim V$.

The set of all linear maps $A : U \rightarrow V$ has a natural vector space structure under pointwise addition and scalar multiplication, so

$$(A_1 + A_2)(u) := A_1 u + A_2 u, \quad (\lambda A)(u) = \lambda(Au)$$

for all linear maps $A_1, A_2, A : U \rightarrow V$ and all $u \in U$ and $\lambda \in \mathbb{C}$. We denote this vector space $\text{Hom}(U, V)$. It is easy to check that $\dim \text{Hom}(U, V) = \dim U \dim V$. We also denote $\text{Hom}(U, U)$ by $\text{End}(U)$. The vector space $\text{Hom}(U, \mathbb{C})$ is also denoted U^* and called the dual vector space of U .

Suppose U, V, W are three finite dimensional complex vector spaces. A map $b : U \times V \rightarrow W$ is called *bilinear* if for fixed $v \in V$ the map $U \rightarrow W$, $u \mapsto b(u, v)$ is linear, and likewise for fixed $u \in U$ the map $V \rightarrow W$, $v \mapsto b(u, v)$ is linear. The *tensor product* of the vector spaces U and V is a vector space $U \otimes V$ together with a bilinear map $i : U \times V \rightarrow U \otimes V$, also denoted $i(u, v) = u \otimes v$ for $u \in U$ and $v \in V$, such that for each bilinear map $b : U \times V \rightarrow W$ to a third vector space W there exists a unique linear map $B : U \otimes V \rightarrow W$ with $b(u, v) = B(u \otimes v)$ for all $u \in U$ and $v \in V$. The linear map B is called the *lift* of the bilinear map b (from the direct product $U \times V$ to the tensor product $U \otimes V$). The uniqueness of the linear map B implies that the cone $\{u \otimes v; u \in U, v \in V\}$ of pure tensors in $U \otimes V$ spans the vector space $U \otimes V$. Here we use the word *cone* for a subset of a vector space, that is invariant under scalar multiplication.

The tensor product is unique up to natural isomorphism. Indeed, if $U \boxtimes V$ is another tensor product with associated bilinear map $j : U \times V \rightarrow U \boxtimes V$ and $j(u, v) = u \boxtimes v$ then there exist unique linear lifts

$$J : U \otimes V \rightarrow U \boxtimes V, \quad J(u \otimes v) = u \boxtimes v$$

of $j : U \times V \rightarrow U \boxtimes V$ and

$$I : U \boxtimes V \rightarrow U \otimes V, I(u \boxtimes v) = u \otimes v$$

of $i : U \times V \rightarrow U \otimes V$, and so $IJ = \text{id}_{U \otimes V}$ and $JI = \text{id}_{U \boxtimes V}$. Hence I and J are inverses of each other.

For the existence of the tensor product we can take for $U \otimes V$ the free vector space $F(U \times V)$ on the set $U \times V$ modulo the linear subspace of $F(U \times V)$ spanned by the elements

$$\begin{aligned} &(u_1 + u_2, v) - (u_1, v) - (u_2, v), (\lambda u, v) - \lambda(u, v) \\ &(u, v_1 + v_2) - (u, v_1) - (u, v_2), (u, \lambda v) - \lambda(u, v) \end{aligned}$$

for all $u_1, u_2, u \in U, v_1, v_2, v \in V$ and $\lambda \in \mathbb{C}$.

If $A \in \text{End}(U)$ and $B \in \text{End}(V)$ then $A \otimes B \in \text{End}(U \otimes V)$ is defined by $(A \otimes B)(u \otimes v) = A(u) \otimes B(v)$ for all $u \in U$ and $v \in V$. If $A_1, A_2 \in \text{End}(U)$ and $B_1, B_2 \in \text{End}(V)$ then clearly $(A_1 \otimes B_1)(A_2 \otimes B_2) = (A_1 A_2) \otimes (B_1 B_2)$.

The bilinear map $U^* \times V \rightarrow \text{Hom}(U, V)$ sending the pair (f, v) to the linear map $u \mapsto f(u)v$ lifts to a linear map $U \otimes V \rightarrow \text{Hom}(U, V)$ sending the pure tensor $f \otimes v$ to the linear map $u \mapsto f(u)v$. It is easy to see that this linear map is a linear isomorphism, and so we have a natural isomorphism $U^* \otimes V \cong \text{Hom}(U, V)$.

The tensor product of vector spaces is associative in the sense that the linear spaces $(U \otimes V) \otimes W$ and $U \otimes (V \otimes W)$ are naturally isomorphic. Likewise $(A \otimes B) \otimes C \cong A \otimes (B \otimes C)$ on $(U \otimes V) \otimes W \cong U \otimes (V \otimes W)$ for $A \in \text{End}(U)$, $B \in \text{End}(V)$ and $C \in \text{End}(W)$. The *tensor algebra* TV on the vector space V is defined as the graded direct sum $\bigoplus \text{T}^k V$ with $\text{T}^k V$ inductively defined by $\text{T}^0 V = \mathbb{C}$ and $\text{T}^{k+1} V = \text{T}^k V \otimes V$ for all $k \in \mathbb{N}$. By associativity we have $\text{T}^k V \otimes \text{T}^l V \cong \text{T}^{k+l} V$ for all $k, l \in \mathbb{N}$, and so $\text{TV} = \bigoplus \text{T}^k V$ becomes a graded associative algebra with respect to the tensor product map \otimes as multiplication.

There are two graded ideals $\text{I}_\pm V = \bigoplus \text{I}_\pm^k V$ of TV generated (through left and right multiplications) by the degree two tensors $(v_1 \otimes v_2 \pm v_2 \otimes v_1)$ for all $v_1, v_2 \in V$. The quotient algebras $\text{SV} = \bigoplus \text{S}^k V = \text{TV}/\text{I}_- V$ and $\wedge V = \bigoplus \wedge^k V = \text{TV}/\text{I}_+ V$ are the so called *symmetric algebra* and *exterior algebra* on V respectively. The symmetric algebra SV is commutative for the induced multiplication, and this multiplication is usually suppressed in the notation (like with multiplication in a group). The induced multiplication

on the exterior algebra $\wedge V$ is denoted by \wedge and called the *wedge product*. We have $\alpha \wedge \beta = (-1)^{kl} \beta \wedge \alpha$ for $\alpha \in \wedge^k V$ and $\beta \in \wedge^l V$.

In case $V = U^*$ is the dual space of a vector space U then $T^k V$ can be identified with the space of scalar valued multilinear forms in k arguments from U . Here *multilinear* is used in the sense that, if all arguments except one remain fixed, then the resulting form is linear in that one argument. In turn $SV = PU = \oplus P^k U$ can be identified with the space of polynomial functions on U by restriction to the main diagonal in U^k . Likewise $\wedge^k V = \wedge^k U^*$ can be identified with the space of alternating multilinear forms in k arguments from U . So $\alpha \in \wedge^k U^*$ means that α is multilinear in k arguments from U and $\alpha(u_{\sigma(1)}, \dots, u_{\sigma(k)}) = \varepsilon(\sigma) \alpha(u_1, \dots, u_k)$ for σ in the symmetric group \mathfrak{S}_k .

Exercise 1.1. Show that $(U \otimes V) \otimes W$ and $U \otimes (V \otimes W)$ are naturally isomorphic for U, V, W vector spaces.

Exercise 1.2. Show that for $A \in \text{End}(U)$, $B \in \text{End}(V)$ and so $A \otimes B \in \text{End}(U \otimes V)$ we have $\text{tr}(A \otimes B) = \text{tr}(A)\text{tr}(B)$.

Exercise 1.3. Show that for a vector space V of dimension n one has

$$\dim S^k V = \binom{n+k-1}{k}, \quad \dim \wedge^k V = \binom{n}{k}$$

for all $k \in \mathbb{N}$.

2 Representations of groups

Throughout this section let G be a group and U, V, W finite dimensional vector spaces over the complex numbers.

A *representation* of a group G on a vector space V is a homomorphism $\rho : G \rightarrow \text{GL}(V)$. Note that necessarily V is nonzero. So a representation of G will be given by a pair (ρ, V) with V a finite dimensional vector space, called the representation space, and $\rho : G \rightarrow \text{GL}(V)$ a homomorphism. If $\rho(x) = 1$ for all $x \in G$ then we speak of the *trivial* representation of G on V . A linear subspace U of a representation space V of G is called *invariant* if for all $x \in G$ and all $u \in U$ we have $\rho(x)u \in U$. If in addition U is nonzero then we get a subrepresentation (ρ_U, U) of (ρ, V) defined by $\rho_U(x) = \rho(x)|_U$ for all $x \in G$. Likewise, if U is a proper invariant subspace of V then we get a quotient representation $(\rho_{V/U}, V/U)$ defined by $\rho_{V/U}(x)(v+U) = \rho(x)(v)+U$ for $x \in G$ and $v \in V$.

We say that a representation (ρ, V) of G is *irreducible* if the only two invariant linear subspaces of V are the trivial invariant linear subspaces $\{0\}$ and V . For example, the trivial representation of G on V is irreducible if and only if $\dim V = 1$. If (ρ, V) is a representation of a group G and $H < G$ is a subgroup then by restriction (ρ, V) becomes also a representation of H . This process is called *branching* or *symmetry breaking* from G to H .

Using constructions of linear algebra one can make new representations from old ones. For example, the *outer tensor product* of two representations (ρ_1, V_1) of a group G_1 and (ρ_2, V_2) of a group G_2 . The outer tensor product $\rho_1 \boxtimes \rho_2$ is a representation of the direct product group $G_1 \times G_2$ on the vector space $V_1 \otimes V_2$, and is defined by $(\rho_1 \boxtimes \rho_2)(x_1, x_2) = \rho_1(x_1) \otimes \rho_2(x_2)$ for $x_1 \in G_1$ and $x_2 \in G_2$. If $G_1 = G_2 = G$ then the *inner tensor product* $\rho_1 \otimes \rho_2$ of two representations (ρ_1, V_1) and (ρ_2, V_2) of the same group G is a representation of that group G on $V_1 \otimes V_2$, which is defined by $(\rho_1 \otimes \rho_2)(x) = (\rho_1(x)) \otimes (\rho_2(x))$ for $x \in G$. So the inner tensor product is obtained from the outer tensor product by branching from the direct product group $G \times G$ to the diagonal subgroup G .

If (ρ, V) is a representation of a group G then we also get representations $(S^k \rho, S^k V)$ and $(\wedge^k \rho, \wedge^k V)$ of the same group G , called the symmetric power and the wedge power representations of degree k respectively.

If $A \in \text{Hom}(U, V)$ then the dual linear map $A^* \in \text{Hom}(V^*, U^*)$ will be defined by $(A^*f)u = f(Au)$ for $f \in V^*$ and $u \in U$. It is easy to check that $(BA)^* = A^*B^*$ for $A \in \text{Hom}(U, V)$ and $B \in \text{Hom}(V, W)$. If (ρ, V)

is a representation of a group G then the *dual representation* (ρ^*, V^*) of G is defined by $\rho^*(x) = (\rho(x^{-1}))^*$ for $x \in G$. More generally, if (ρ, V) and (σ, W) are two representations of a group G then the representation $(\text{Hom}(\rho, \sigma), \text{Hom}(V, W))$ of G is defined by $\text{Hom}(\rho, \sigma)(x)A = \sigma(x)A\rho(x^{-1})$ for $x \in G$ and $A \in \text{Hom}(V, W)$.

If (ρ, V) is a representation of a group G then we denote by V^G the linear subspace $\{v \in V; \rho(x)v = v \ \forall x \in G\}$ of V of fixed vectors. For example, for representations (ρ, V) and (σ, W) of G the space $\text{Hom}(V, W)^G$ consists of those $A \in \text{Hom}(V, W)$ for which $A\rho(x) = \sigma(x)A$ for all $x \in G$. Such a linear map $A \in \text{Hom}(V, W)$ is called an *intertwining operator* or simply an *intertwiner* from (ρ, V) to (σ, W) . The two representations (ρ, V) and (σ, W) of G are called *equivalent* if there exists an intertwiner $\text{Hom}(V, W)^G$ which is also a linear isomorphism, and we write $(\rho, V) \sim (\sigma, W)$. The natural isomorphism $\text{Hom}(V, W) \cong V^* \otimes W$ gives an equivalence $\text{Hom}(\rho, \sigma) \sim \rho^* \otimes \sigma$ of representations.

However, in daily life people are sometimes sloppy and use the word representation while equivalence class of representation is meant. Be aware of that.

A representation (ρ, V) of a group G is called *completely reducible* if for any invariant subspace U of V there exists a complementary invariant subspace U^\perp . So $U + U^\perp = V$ and $U \cap U^\perp = \{0\}$, which is also denoted $V = U \oplus U^\perp$, and moreover U^\perp is invariant as well. We denote $\rho = \rho_U \oplus \rho_{U^\perp}$ for this situation (strictly speaking if U, U^\perp are both nonzero).

Suppose the vector space V carries a Hermitian inner product $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{C}$, which by definition is a positive definite sesquilinear form on V , usually linear in the first argument and antilinear in the second argument, and interchange of arguments amounts to complex conjugation. The pair $(V, \langle \cdot, \cdot \rangle)$ is called a finite dimensional *Hilbert space*. A representation (ρ, V) of a group G on a Hilbert space $(V, \langle \cdot, \cdot \rangle)$ is called *unitary* if

$$\langle \rho(x)v_1, \rho(x)v_2 \rangle = \langle v_1, v_2 \rangle$$

for all $x \in G$. So a unitary representation is a triple $(\rho, V, \langle \cdot, \cdot \rangle)$ with $(V, \langle \cdot, \cdot \rangle)$ a Hilbert space and $\rho : G \rightarrow \text{U}(V, \langle \cdot, \cdot \rangle)$ a homomorphism of G into the *unitary group* of that Hilbert space.

Lemma 2.1. *A unitary representation $(\rho, V, \langle \cdot, \cdot \rangle)$ of a group G is always completely reducible.*

Proof. If $U \subset V$ is an invariant subspace then the orthogonal complement $U^\perp = \{v \in V; \langle u, v \rangle = 0 \forall u \in U\}$ is easily seen to be also invariant. \square

Theorem 2.2. *Any representation (ρ, V) of a finite group G is completely reducible.*

Proof. We claim that the representation (ρ, V) is always *unitarizable*, that is can be made unitary for some Hermitian inner product $\langle \cdot, \cdot \rangle$ on V . Just pick any Hermitian inner product $\langle \cdot, \cdot \rangle'$ on V . By averaging over G we obtain a new Hermitian inner product

$$\langle v_1, v_2 \rangle = \frac{1}{|G|} \sum_{x \in G} \langle \rho(x)v_1, \rho(x)v_2 \rangle'$$

and it is easily checked that $\langle \rho(x)v_1, \rho(x)v_2 \rangle = \langle v_1, v_2 \rangle$ for all $x \in G$. So $(\rho, V, \langle \cdot, \cdot \rangle)$ becomes a unitary representation, and we can apply the above lemma. \square

Remark 2.3. *The above theorem has an extension to compact topological groups and continuous finite dimensional representations of such groups. A topological group G is both a topological space and a group, and the two structures are compatible in the sense that multiplication $G \times G \rightarrow G, (x, y) \mapsto xy$ and inversion $G \rightarrow G, x \mapsto x^{-1}$ are continuous maps. Finite groups are compact topological groups relative to the discrete topology, and so any representation of a finite group is automatically continuous. The simplest example of a compact topological group, which is not a finite group, is the circle group $\mathbb{R}/2\pi\mathbb{Z}$. Geometrically $\mathbb{R}/2\pi\mathbb{Z} \cong U_1(\mathbb{C}) \cong SO_2(\mathbb{R})$ is the group of rotations of the complex plane $\mathbb{C} \cong \mathbb{R}^2$ around the origin.*

It is a nontrivial theorem of John von Neumann (1903-1957) that for any compact topological group G there exists a positive measure μ that is invariant under left and right multiplications. Such a measure μ on G assigns to a continuous function $f : G \rightarrow \mathbb{C}$ by integration against μ a complex number

$$\int_G f(x) d\mu(x)$$

which is positive if f is positive and satisfies the invariance relations

$$\int_G f(xy) d\mu(x) = \int_G f(yx) d\mu(x) = \int_G f(x) d\mu(x)$$

for all $y \in G$. Moreover, such a measure becomes unique by the normalization $\int_G d\mu(x) = 1$. For the circle group $\mathbb{R}/2\pi\mathbb{Z}$ with standard coordinate θ this normalized invariant measure is just

$$\frac{1}{2\pi} \int_0^{2\pi} f(\theta) d\theta$$

the usual Riemann integral. Now the proof of the above theorem carries verbatim over to the present situation by using

$$\langle v_1, v_2 \rangle = \int_G \langle \rho(x)v_1, \rho(x)v_2 \rangle' d\mu(x)$$

in stead of the finite normalized sum as above.

The conclusion is that the representation theory of finite (or even compact) groups boils down to two fundamental problems. In the first place classify the equivalence classes of irreducible representations and preferably give constructions and nice models for each of them. In the second place decompose a given representation into irreducible ones.

An easy but important result is Schur's lemma, which was found by Issai Schur (1875-1941) in 1905.

Lemma 2.4. *If (ρ, U) is an irreducible representation of a group G then the vector space $\text{End}(U)^G$ of self intertwiners for (ρ, U) consists only of scalar linear maps. If (ρ, U) and (σ, V) are both irreducible representations of G then either $\dim \text{Hom}(U, V)^G$ is equal to 1 if $(\rho, U) \sim (\sigma, V)$ or is equal to 0 if $(\rho, U) \not\sim (\sigma, V)$.*

Proof. Suppose $A \in \text{End}(U)^G$ is a self intertwiner for (ρ, U) . Since scalars are self intertwiners we also have $(A - \lambda) \in \text{End}(U)^G$ for all $\lambda \in \mathbb{C}$. If λ is an eigenvalue of A then the eigenspace $\ker(A - \lambda)$ is a nonzero invariant subspace of U and so equal to U itself by irreducibility of (ρ, U) . Hence $A = \lambda$ for some $\lambda \in \mathbb{C}$ and the first statement follows.

Suppose $A \in \text{Hom}(U, V)^G$ is a nonzero intertwiner. Then $\ker A$ is a proper invariant subspace of U and so is equal to $\{0\}$ since (ρ, U) is irreducible. Also $\text{im } A$ is a nonzero invariant subspace of V and so is equal to V since (σ, V) is irreducible. Hence any nonzero intertwiner $A \in \text{Hom}(U, V)^G$ is a linear isomorphism and so gives an equivalence $(\rho, U) \sim (\sigma, V)$ of representations.

If $A, B \in \text{Hom}(U, V)^G$ with $A \neq 0$ then $BA^{-1} \in \text{End}(V)^G$ is a self intertwiner for (σ, V) . Hence $BA^{-1} = \lambda$ for some $\lambda \in \mathbb{C}$ and so $B = \lambda A$,

which implies $\dim \text{Hom}(U, V)^G = 1$. On the other hand, if $(\rho, U) \approx (\sigma, V)$ then clearly $\dim \text{Hom}(U, V)^G = 0$. \square

Corollary 2.5. *An irreducible representation of an Abelian group is one dimensional.*

Proof. Suppose (ρ, V) is an irreducible representation of an Abelian group G . Then all linear operators $\rho(x)$ for $x \in G$ are self intertwiners, and hence scalars by Schur's lemma. Hence any linear subspace of V is invariant and therefore $\dim V = 1$ by the definition of irreducibility. \square

Exercise 2.1. *Check that a positive linear combination of Hermitian inner products on a vector space V is again a Hermitian inner product.*

Exercise 2.2. *Let B_n be the subgroup of the general linear group $\text{GL}_n(\mathbb{C})$ of upper triangular matrices, so $A = (a_{ij}) \in B_n$ if and only if $a_{ij} = 0$ for $i > j$. Show that the natural representation of B_n on \mathbb{C}^n is not completely reducible for $n \geq 2$.*

Exercise 2.3. *In this section all vector spaces were finite dimensional and over the complex numbers \mathbb{C} . Show that Schur's lemma does not hold over the real numbers \mathbb{R} by looking at the real representation of the circle group*

$$\mathbb{R}/2\pi\mathbb{Z} \rightarrow \text{GL}_2(\mathbb{R}), \theta \mapsto \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

by rotations of the real plane \mathbb{R}^2 .

3 Character theory for finite groups

If V is a finite dimensional vector space with basis e_i then the *trace* $\text{tr} A$ of a linear map $A : V \rightarrow V$, with matrix (a_{ij}) given by $Ae_j = \sum_i a_{ij}e_i$, is defined by $\text{tr} A = \sum_i a_{ii}$. One easily checks that $\text{tr}(AB) = \text{tr}(BA)$ for all $A, B \in \text{End}(V)$ and in particular $\text{tr}(BAB^{-1}) = \text{tr} A$ in case $\det B \neq 0$. In turn this implies that $\text{tr} A$ is well defined, independent of the chosen basis.

Suppose G is a group and (ρ, V) a finite dimensional representation. The *character* $\chi_\rho : G \rightarrow \mathbb{C}$ of (ρ, V) is defined by

$$\chi_\rho(x) = \text{tr} \rho(x)$$

for $x \in G$. For finite groups we will show that the character of a finite dimensional representation characterizes the representation upto equivalence, which explains the terminology character.

We list some simple properties of characters. Suppose (ρ, V) and (σ, W) are both representations of G . Clearly $\chi_\rho = \chi_\sigma$ if $(\rho, V) \sim (\sigma, W)$. It is also clear that $\chi_\rho(yxy^{-1}) = \chi_\rho(x)$ for all $x, y \in G$ and so characters are constant on conjugation classes of G . It is also obvious that $\chi_\rho(e) = \dim V$. Finally

$$\chi_{\rho \oplus \sigma}(x) = \chi_\rho(x) + \chi_\sigma(x), \chi_{\rho \otimes \sigma}(x) = \chi_\rho(x)\chi_\sigma(x)$$

and (the second equality sign only for G a finite group)

$$\chi_{\rho^*}(x) = \chi_\rho(x^{-1}) = \overline{\chi_\rho(x)}$$

for all $x \in G$.

From now on we shall assume that G is a *finite* group. Let $L(G)$ denote the vector space of complex valued functions on G . For $\phi, \psi \in L(G)$ we define an Hermitian inner product

$$\langle \phi, \psi \rangle = \frac{1}{|G|} \sum_{x \in G} \phi(x) \overline{\psi(x)}$$

turning $L(G)$ into a finite dimensional Hilbert space. The linear subspace of class functions in $L(G)$, that is functions constant on conjugation classes, is denoted $C(G)$. So characters of representations of G are elements of $C(G)$.

The next theorem states the so called Schur orthogonality relations for the irreducible characters of G . The proof is a beautiful application of Schur's lemma, and was in fact the principal motivation for Schur to come up with his lemma.

Theorem 3.1. *If (ρ, V) and (σ, W) are irreducible representations of a finite group G then*

$$\langle \chi_\rho, \chi_\sigma \rangle = \delta_{\rho\sigma}$$

with the Kronecker delta notation $\delta_{\rho\sigma} = 1$ if $\rho \sim \sigma$ and $\delta_{\rho\sigma} = 0$ if $\rho \not\sim \sigma$.

Proof. Let (τ, U) be an arbitrary representation of G , and let U^G be the space of fixed vectors for G in U . Define the linear map

$$P : U \rightarrow U, Pu = \frac{1}{|G|} \sum_{x \in G} \tau(x)u$$

for $u \in U$. Then $\tau(x)P = P$ for all $x \in G$ and hence $P^2 = P$. So P is a linear projection operator with image $\text{im } P = U^G$. In turn this implies

$$\langle \chi_\tau, 1 \rangle = \frac{1}{|G|} \sum_{x \in G} \text{tr}(\tau(x)) = \text{tr}(P) = \dim U^G$$

as the trace is a linear form and the trace of a linear projection operator is the dimension of its image.

If (ρ, V) and (σ, W) are irreducible representations of G then we shall apply the above formula to the representation $\tau = \text{Hom}(\rho, \sigma) \sim \rho^* \otimes \sigma$ on the vector space $U = \text{Hom}(V, W) \cong V^* \otimes W$ as defined by $\tau(x)A = \sigma(x)A\rho(x^{-1})$ for $x \in G$ and $A \in \text{Hom}(V, W)$. Since by Schur's lemma the space of intertwiners $U^G = \text{Hom}(V, W)^G$ has dimension $\delta_{\rho\sigma}$ we get

$$\langle \chi_\sigma, \chi_\rho \rangle = \langle \chi_{\rho^* \otimes \sigma}, 1 \rangle = \langle \chi_{\text{Hom}(\rho, \sigma)}, 1 \rangle = \delta_{\rho\sigma}$$

and the Schur orthogonality relations follow from $\langle \chi_\rho, \chi_\sigma \rangle = \overline{\delta_{\rho\sigma}} = \delta_{\rho\sigma}$. \square

Suppose (ρ, V) is a representation of G , which by complete reducibility can be written $(\rho_1 \oplus \dots \oplus \rho_m, V_1 \oplus \dots \oplus V_m)$ as a direct sum of irreducibles. Let (σ, W) be an irreducible representation of G . Then the number of irreducible components (ρ_i, V_i) in (ρ, V) equivalent to (σ, W) is equal to $\langle \chi_\rho, \chi_\sigma \rangle \in \mathbb{N}$ and is called the *multiplicity* of (σ, W) in (ρ, V) . The characters of the irreducible representations of G are called the irreducible characters of G .

Corollary 3.2. *Two representations of a finite group G with equal characters are equivalent, and so the character characterizes a representation upto equivalence.*

Remark 3.3. *The Schur orthogonality relations have a natural extension from finite to compact groups. Indeed, let G be a compact group with μ the normalized invariant measure on the space $L(G)$ of continuous functions on G . If (ρ, V) and (σ, W) are irreducible representations of G then we have*

$$\langle \chi_\rho, \chi_\sigma \rangle = \delta_{\rho\sigma}$$

relative to the Hermitian inner product

$$\langle \phi, \psi \rangle = \int_G \phi(x) \overline{\psi(x)} d\mu(x)$$

of $\phi, \psi \in L(G)$.

For example, the circle group $\mathbb{R}/2\pi\mathbb{Z}$ has irreducible representations

$$\rho_n : \mathbb{R}/2\pi\mathbb{Z} \rightarrow \mathrm{GL}_1(\mathbb{C}) = \mathbb{C}^\times, \rho_n(\theta) = e^{in\theta}$$

indexed by $n \in \mathbb{Z}$. The Schur orthogonality relations amount to

$$\frac{1}{2\pi} \int_0^{2\pi} \rho_m(\theta) \overline{\rho_n(\theta)} d\theta = \frac{1}{2\pi} \int_0^{2\pi} e^{im\theta} e^{-in\theta} d\theta = \frac{1}{2\pi} \int_0^{2\pi} e^{i(m-n)\theta} d\theta = \delta_{mn}$$

for $m, n \in \mathbb{Z}$ which are familiar from Fourier analysis. It is known from Fourier analysis that the space of Fourier polynomials is dense in $L^2(\mathbb{R}/2\pi\mathbb{Z})$ which in turn implies that each irreducible representation of $\mathbb{R}/2\pi\mathbb{Z}$ is equal to ρ_n for some $n \in \mathbb{Z}$.

As before let us assume that G is a finite group. If $\phi \in L(G)$ and (ρ, V) is a representation of G then the linear operator

$$\rho(\phi) = \frac{1}{|G|} \sum_{x \in G} \phi(x) \rho(x) \in \mathrm{End}(V)$$

has trace equal to $\mathrm{tr} \rho(\phi) = \langle \phi, \chi_{\rho^*} \rangle$. If $\phi \in C(G)$ is a class function on G then it is easy to check that $\rho(\phi) \in \mathrm{End}(V)^G$ is an intertwiner. If in addition (ρ, V) is irreducible then $\rho(\phi)$ is a scalar by Schur's lemma. It follows by taking traces that this scalar is equal to $\langle \phi, \chi_{\rho^*} \rangle / \dim V$. Hence if $\phi \in C(G)$ is orthogonal to all irreducible characters of G then by complete reducibility $\rho(\phi) = 0$ for any representation (ρ, V) of G .

Theorem 3.4. *The irreducible characters form an orthonormal basis of $C(G)$ with respect to the standard Hermitian inner product $\langle \cdot, \cdot \rangle$.*

Proof. The left regular representation λ of G on the vector space $L(G)$ is defined by $(\lambda(x)\phi)(y) = \phi(x^{-1}y)$ for $x, y \in G$. The functions $\delta_x \in L(G)$ for $x \in G$ are defined by $\delta_x(y) = \delta_{xy}$ for $x, y \in G$ and form a basis of $L(G)$ since $\phi = \sum_x \phi(x)\delta_x$ for all $\phi \in L(G)$. Since $\lambda(x)\delta_y = \delta_{xy}$ for $x, y \in G$ we get $\phi = \sum_x \phi(x)\lambda(x)\delta_e = |G|\lambda(\phi)\delta_e$ for $\phi \in L(G)$.

Let $\phi \in C(G)$ be a class function which is orthogonal to all irreducible characters of G . Then $\rho(\phi) = 0$ for any representation (ρ, V) of G . Taking (ρ, V) equal to the left regular representation $(\lambda, L(G))$ we conclude that $\lambda(\phi) = 0$. Hence $\phi = |G|\lambda(\phi)\delta_e = 0$ and so the result follows. \square

The dimension of the space $C(G)$ of class functions is equal to the number of conjugation classes in G . Hence the number of equivalence classes of irreducible representations of G is equal to the number of conjugation classes in G .

Example 3.5. *The four group (in German Vierergruppe) V_4 of Klein is a group with a unit element e and three involutions a, b, c which in turn implies $ab = ba = c, bc = cb = a, ca = ac = b$. The character table is a matrix of the form*

V_4	e	a	b	c
χ_1	1	1	1	1
χ_2	1	1	-1	-1
χ_3	1	-1	1	-1
χ_4	1	-1	-1	1

where the rows are indexed by the irreducible characters and the columns are indexed by representatives of the conjugation classes. The matrix element is the value of the irreducible character at the conjugation class.

Example 3.6. *The symmetric group \mathfrak{S}_4 on 4 letters has character table*

\mathfrak{S}_4	e	(12)	(12)(34)	(123)	(1234)
χ_1	1	1	1	1	1
χ_2	1	-1	1	1	-1
χ_3	2	0	2	-1	0
χ_4	3	1	-1	0	-1
χ_5	3	-1	-1	0	1

with χ_1 the trivial character, χ_2 the sign character ε , χ_3 the lift from the two dimensional irreducible character of \mathfrak{S}_3 via the isomorphism $\mathfrak{S}_4/V_4 \cong \mathfrak{S}_3$,

χ_4 the character of the representation ρ_4 via reflections and rotations of the tetrahedron and $\chi_5 = \chi_2\chi_4$ the character of the representation $\rho_5 = \varepsilon \otimes \rho_4$ of \mathfrak{S}_4 . In order to do Hermitian inner product calculations with characters one should check that the conjugation classes have 1, 6, 3, 8, 6 elements respectively.

Example 3.7. The alternating group \mathfrak{A}_5 on 5 letters has 5 conjugation classes with representatives the unit e , $a = (12)(34)$, $b = (123)$, $c = (12345)$, $d = (13524)$ and with 1, 15, 20, 12, 12 elements respectively. The icosahedron has 12 vertices, 30 edges and 20 faces in accordance with Euler's formula $12 - 30 + 20 = 2$. The 15 lines through midpoints of opposite edges fall apart in 5 orthogonal triples, giving an isomorphism from the rotation group of the icosahedron onto \mathfrak{A}_5 . The class of a consists of order 2 rotations around any of these 15 lines. The class of b consists of order 3 rotations, 2 around any line through midpoints of opposite faces, so altogether 20. The rotations of order 5 around the lines through opposite vertices fall into 2 classes of equal size, namely 2 rotations over $2\pi/5$ and 2 rotations over $4\pi/5$ for each of these 6 lines. The character table of \mathfrak{A}_5 becomes

\mathfrak{A}_5	e	a	b	c	d
χ_1	1	1	1	1	1
χ_2	3	-1	0	τ	τ'
χ_3	3	-1	0	τ'	τ
χ_4	4	0	1	-1	-1
χ_5	5	1	-1	0	0

with $\tau = (1 + \sqrt{5})/2$ the golden ratio and $\tau' = (1 - \sqrt{5})/2 = -1/\tau$. These two numbers are the roots of the equation $x^2 - x - 1 = 0$. The representation ρ_2 via rotations of the icosahedron has character χ_2 and ρ_3 is its Galois conjugate. The representation ρ_4 with character χ_4 is just the restriction of the reflection representation from \mathfrak{S}_5 to \mathfrak{A}_5 while $\chi_2\chi_3 = \chi_4 + \chi_5$.

Exercise 3.1. Show that the character of the left regular representation of a finite group G is equal to $|G|\delta_e$. Show that each irreducible representation of G occurs in the left regular representation with multiplicity equal to the dimension of that irreducible representation. Conclude that the sum of the squares of the dimensions of the irreducible representations is equal to the order of the group.

Exercise 3.2. Let $Q = \{\pm 1, \pm i, \pm j, \pm k\} \subset \text{SL}_2(\mathbb{C})$ with

$$1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, i = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, j = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, k = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.$$

Check that the relations

$$i^2 = j^2 = k^2 = -1, ij = -ji = k, jk = -kj = i, ki = -ik = j$$

hold and conclude that Q is a subgroup of $\text{SL}_2(\mathbb{C})$, the so called quaternion group. Show that $Q/\{\pm 1\} \cong V_4$. Determine the conjugation classes in Q . Find the character table of Q .

Exercise 3.3. Show that an irreducible character of a finite direct product group $G_1 \times G_2$ is of the form $\chi_1 \times \chi_2(x, y) = \chi_1(x)\chi_2(y)$ with χ_1 an irreducible character of G_1 and χ_2 an irreducible character of G_2 .

Exercise 3.4. Show that the irreducible characters of the group $\mathfrak{A}_5 \times \{\pm 1\}$ of reflections and rotations of the icosahedron are of the form

$$\chi_{\pm}(x, 1) = \chi(x), \chi_{\pm}(x, -1) = \pm\chi(x)$$

for $x \in \mathfrak{A}_5$ and χ an irreducible character of \mathfrak{A}_5 .

Exercise 3.5. Show that a representation (ρ, V) of a finite (or even compact) group G is irreducible if its character $\chi \in \mathbb{C}(G)$ has norm 1 for the standard Hermitian inner product on $L(G)$.

4 Molecular vibrations after Wigner

Consider a molecule M in \mathbb{R}^3 with n atoms numbered $1, \dots, n$. Suppose that $q = (q_1, \dots, q_n) \in \mathbb{R}^{3n}$ is an equilibrium position of M with $q_i \in \mathbb{R}^3$ the position of the atom with number i . We consider small deviations $x = (x_1, \dots, x_n) \in \mathbb{R}^{3n}$ in time t from the stationary equilibrium position q , and so M is in position $q + x$. The kinetic energy K of this deviation $x = x(t)$ is equal to

$$K(\dot{x}) = (\dot{x}|\dot{x})/2$$

with $(x|y) = ((x_1, \dots, x_n)|(y_1, \dots, y_n)) = \sum_i m_i(x_i, y_i)$ with m_i the mass of the atom with number i and (\cdot, \cdot) the standard inner product on \mathbb{R}^3 . The potential energy V is in harmonic approximation a homogeneous quadratic polynomial

$$V(x) = (x|Hx)/2$$

with $H : \mathbb{R}^{3n} \rightarrow \mathbb{R}^{3n}$ a symmetric operator relative to $(\cdot|\cdot)$, that is $(Hx|y) = (x|Hy)$ for all $x, y \in \mathbb{R}^{3n}$. Indeed, we may assume $V(0) = 0$ because the potential is determined from the conservative force field $F : \mathbb{R}^{3n} \rightarrow \mathbb{R}^{3n}$ by the equation $F(x) = -\nabla V(x)$. The linear part of V vanishes because $x = 0$ is an equilibrium position and so $F(0) = 0$. Cubic and higher order terms of V are ignored because x is small. Equivalently, the force field $F(x) = -Hx$ is a linear vector field. The equation of motion becomes

$$\ddot{x} + Hx = 0$$

by Newton's law.

Define the translation subspace T and the rotation subspace R of \mathbb{R}^{3n} by

$$\begin{aligned} T &= \{(u, \dots, u) \in \mathbb{R}^{3n}; u \in \mathbb{R}^3\} \\ R &= \{(v \times q_1, \dots, v \times q_n); v \in \mathbb{R}^3\} \end{aligned}$$

with \times the vector product on \mathbb{R}^3 . If we assume that the potential energy V is invariant under translations and rotations of M as a whole, that is there are no external forces on M , then $V(x) = 0$ for $x \in T + R$. If we assume that M is not collinear then it can be shown that $\dim R = 3$ and $T \cap R = \{0\}$, and so we have an orthogonal direct sum decomposition

$$\mathbb{R}^{3n} = V \oplus T \oplus R$$

with V the so called internal vibration space of dimension $3n - 6$. Since $H = 0$ on $T + R$ and H is symmetric we have $H(V) \subset V$.

Finally we assume that q is a stable equilibrium position of M . This means that all eigenvalues of H on V are strictly positive, and the square roots of these eigenvalues are the *frequencies* of the eigenvibrations, after reduction of translation and rotation symmetry. In general all eigenvalues of H on V have multiplicity one, in which case one measures $(3n - 6)$ different frequencies. However eigenspaces of H on V might have dimension ≥ 2 , in which case one speaks of (spectral) *degeneration*. The principal cause for degeneration is *symmetry* of M .

Suppose that the atoms with number i and number j are of the same kind if and only if $m_i = m_j$. If the center of gravity $\sum m_i q_i / \sum m_i$ of M is taken at the origin of \mathbb{R}^3 then the symmetry group G of M in equilibrium position $q = (q_1, \dots, q_n) \in \mathbb{R}^{3n}$ is given by

$$G = \{a \in O(\mathbb{R}^3); \forall i \exists j \text{ with } m_i = m_j \text{ and } a q_i = q_j\}.$$

As subgroup of $O(\mathbb{R}^3)$ the group G has a standard representation π on \mathbb{R}^3 and we write $\chi(a) = \text{tr } a$ for its character. There is a natural homomorphism $G \rightarrow \mathfrak{S}_n, a \mapsto \sigma_a$ given by $\sigma_a(i) = j$ if and only if $a q_i = q_j$. We are now able to define the vibration representation Π from G on the total vibration space \mathbb{R}^{3n} by

$$\Pi(a)(x_1, \dots, x_n) = (a x_{\sigma_a^{-1}(1)}, \dots, a x_{\sigma_a^{-1}(n)})$$

for $a \in G$ and $x \in \mathbb{R}^{3n}$. Indeed, one thinks of $x = (x_1, \dots, x_n) \in \mathbb{R}^{3n}$ as a set of arrows $x_j \in \mathbb{R}^3$ with begin point q_j and for $a \in G$ the new arrow from $\Pi(a)x \in \mathbb{R}^{3n}$ with begin point $q_j = a q_i$ is just $a x_i \in \mathbb{R}^3$. The next theorem is called Wigner's rule.

Theorem 4.1. *The character X of the vibration representation Π of the symmetry group G of the molecule M on the total vibration space \mathbb{R}^{3n} is given by*

$$X(a) = |\{i; \sigma_a(i) = i\}| \cdot \chi(a)$$

for $a \in G$.

Proof. Just think of the $3n \times 3n$ matrix $\Pi(a)$ with scalar entries as a $n \times n$ matrix with entries from $\text{End}(\mathbb{R}^3)$. The matrix $\Pi(a)$ has on the main diagonal place (i, i) the entry $\pi(a)$ from $O(\mathbb{R}^3)$ if and only if $\sigma_a(i) = i$ and 0 otherwise. Hence Wigner's rule is obvious. \square

It is easy to check that the direct sum decomposition $\mathbb{R}^{3n} = V \oplus T \oplus R$ is invariant for the representation Π of G , and in fact we have

$$\Pi = \Pi_V \oplus \Pi_T \oplus \Pi_R \sim \Pi_V \oplus \pi \oplus (\det \otimes \pi).$$

Indeed $\Pi_T \sim \pi$ is obvious, while $\Pi_R \sim \det \otimes \pi$ follows from $a(u \times v) = \det(a)(au \times av)$ for all $a \in O(\mathbb{R}^3)$ and $u, v \in \mathbb{R}^3$. Hence the character

$$X_V = X - \chi - \det \cdot \chi$$

of the internal vibration representation Π_V can be computed using Wigner's rule.

Since the potential energy V is invariant under G , that is since we have $V(\Pi(a)x) = V(x)$ for all $a \in G$ and $x \in \mathbb{R}^{3n}$, we get the commutation relation

$$\Pi(a)H = H\Pi(a)$$

for all $a \in G$. In other words H is an intertwiner for Π . This means that the eigenvalue decomposition

$$V = \bigoplus_{\nu} V_{\nu} = \bigoplus_{\nu} \{v \in V; Hv = \nu^2 v\}$$

is invariant under Π . If the subrepresentation Π_{ν} on V_{ν} is irreducible for all $\nu > 0$ then we say that the operator H_V on V has *natural degeneration* for G . If V_{ν} is reducible for some $\nu > 0$ then we speak of *accidental degeneration*. Accidental degeneration might hint at a larger *hidden* symmetry group.

Let us discuss the example of the methane molecule CH_4 with a carbon atom at the origin and four hydrogen atoms at the four vertices $(1, 1, 1)$, $(1, -1, -1)$, $(-1, 1, -1)$, $(-1, -1, 1)$ of a tetrahedron. The symmetry group G is the reflection and rotation group of the tetrahedron and is isomorphic to \mathfrak{S}_4 .

From the character table of \mathfrak{S}_4 one gets the table

\mathfrak{S}_4	e	(12)	(12)(34)	(123)	(1234)
$ \cdot $	1	6	3	8	6
χ_1	1	1	1	1	1
$\det = \chi_2$	1	-1	1	1	-1
χ_3	2	0	2	-1	0
$\chi = \chi_4$	3	1	-1	0	-1
χ_5	3	-1	-1	0	1
X	15	3	-1	0	-1
X_V	9	3	1	0	-1

which in turn implies

$$\begin{aligned}
\langle X_V, \chi_1 \rangle &= (1 \cdot 9 \cdot 1 + 6 \cdot 3 \cdot 1 + 3 \cdot 1 \cdot 1 + 8 \cdot 0 \cdot 1 + 6 \cdot -1 \cdot 1) / 24 = 1 \\
\langle X_V, \chi_2 \rangle &= (1 \cdot 9 \cdot 1 + 6 \cdot 3 \cdot -1 + 3 \cdot 1 \cdot 1 + 8 \cdot 0 \cdot 1 + 6 \cdot -1 \cdot -1) / 24 = 0 \\
\langle X_V, \chi_3 \rangle &= (1 \cdot 9 \cdot 2 + 6 \cdot 3 \cdot 0 + 3 \cdot 1 \cdot 2 + 8 \cdot 0 \cdot -1 + 6 \cdot -1 \cdot 0) / 24 = 1 \\
\langle X_V, \chi_4 \rangle &= (1 \cdot 9 \cdot 3 + 6 \cdot 3 \cdot 1 + 3 \cdot 1 \cdot -1 + 8 \cdot 0 \cdot 0 + 6 \cdot -1 \cdot -1) / 24 = 2 \\
\langle X_V, \chi_5 \rangle &= (1 \cdot 9 \cdot 3 + 6 \cdot 3 \cdot -1 + 3 \cdot 1 \cdot -1 + 8 \cdot 0 \cdot 0 + 6 \cdot -1 \cdot 1) / 24 = 0
\end{aligned}$$

and hence

$$X_V = \chi_1 + \chi_3 + 2\chi_4.$$

The conclusion is that the internal vibration spectrum of methane in case of natural degeneration has 4 frequencies, one mode transforming under ρ_1 and with multiplicity $\dim \rho_1 = 1$, one mode transforming under ρ_3 with multiplicity $\dim \rho_3 = 2$ and two modes transforming under ρ_4 with multiplicity $\dim \rho_4 = 3$.

The symmetry results of this section give only qualitative information about the nature of spectral degeneration. For finer quantitative information about the location of the spectral lines one needs the further knowledge about the masses m_i and the Hessian H of the potential.

Remark 4.2. *Usually in representation theory one considers representations on complex vector spaces. However, in this section we have tacitly worked with representations on real vector spaces. So some care is required with the concept of irreducible characters over \mathbb{R} or \mathbb{C} , in the sense that a real irreducible character can be either a complex irreducible character or a sum of a complex irreducible character and its complex conjugate. However, in the two examples discussed in this section, the group of reflections and rotations of the tetrahedron (in the case of methane) or the icosahedron (in the case of the buckyball) all complex irreducible characters are real valued, and real irreducible characters are complex irreducible characters as well.*

In fact, problems of this kind would only arise with the cyclic group C_m of order m as symmetry group for $m \geq 3$. But in that case one automatically has the embracing dihedral group D_m of order $2m$ as larger symmetry group of the real molecule M . One can check that complex irreducible characters for D_m are again real valued, and real irreducible characters are complex irreducible characters as well.

Symmetry arguments also give so called *selection rules*. If one shines light on the molecule M with vibrations of M as a result then only light of particular wave length is absorbed in accordance with the particular frequencies $\nu > 0$ of M (or equivalently with particular eigenvalues ν^2 of the symmetric operator H on V). If the spectrum has natural degeneration, then to each frequency ν one associates the irreducible representation ρ_ν of G on the eigenspace V_ν of H on V .

In ordinary spectroscopy one will only see those frequencies ν of M for which the irreducible representation ρ_ν occurs as a subrepresentation of the standard representation ρ of G on \mathbb{R}^3 . This ordinary spectrum is usually seen in infrared. There is also the so called Raman spectrum, which sees only those frequencies ν for which the irreducible representation ρ_ν occurs as subrepresentation of the second symmetric power $S^2\rho$ of the standard representation ρ of G on \mathbb{R}^3 . The Raman spectrum is a second order scattering effect, and is usually seen in ultraviolet. For the mathematics behind these selection rules see the text book Shlomo Sternberg, Group theory and physics, Cambridge University Press, 1994.

The results of this section were obtained by Eugene Wigner (1902-1995) in 1930. In the nineteen twenties and thirties Wigner made various significant applications of representation theory of groups to physics, for which he was awarded the Nobel prize in physics in 1963.

Exercise 4.1. *Show that the dimension of the rotation subspace R of \mathbb{R}^{3n} is equal to 3 if $\text{rk}\{q_1, \dots, q_n\} \geq 2$. Show that $T \cap R = \{0\}$ if q_1, \dots, q_n are not collinear.*

Exercise 4.2. *Show that for a molecule M whose symmetry group G contains the central inversion -1 the ordinary spectrum and the Raman spectrum are disjoint (under the usual assumption of natural degeneration).*

Exercise 4.3. *For $G < O_3(\mathbb{R})$ a finite group let π denote the standard three dimensional representation and χ its character. For $u \in \mathbb{R}^3$ let $L(u)$ be the skew symmetric linear operator on \mathbb{R}^3 defined by $L(u)v = u \times v$. Show that L is an intertwiner from $\det \otimes \pi$ to $\wedge^2 \pi$ and conclude that the character of $S^2 \pi$ is equal to $(\chi - \det)\chi$.*

Exercise 4.4. *The buckyball C_{60} is a molecule with 60 carbon atoms at the vertices of a truncated icosahedron. The symmetry group of the buckyball is the reflection and rotation group of the icosahedron and is isomorphic to*

$\mathfrak{A}_5 \times \{\pm 1\}$. Show that the character X of the natural representation Π of the symmetry group $G \cong \mathfrak{A}_5 \times \{\pm 1\}$ of the buckyball on the total vibration space \mathbb{R}^{180} takes the value 180 at the identity element e , the value 4 at the class of the reflection $-a$ and the value 0 otherwise. If $\psi = \sum \chi_{i,+} + \sum \chi_{i,-}$ in the notation of Exercise 3.4 then check that $\psi(e) = 32$ and $\psi(-a) = 0$. Show that $\langle X, \psi \rangle = 48$ and conclude that the internal vibration spectrum of C_{60} in case of natural degeneration has 46 frequencies. Show that the ordinary spectrum of C_{60} has only 4 frequencies, while the Raman spectrum has 10 frequencies.

The German-Canadian physicist and physical chemist Gerhard Herzberg (1904-1999), who won the Nobel prize for Chemistry in 1971, wrote in the nineteen fifties a highly influential four volume text book *Molecular Spectra and Molecular Structure*, sometimes referred to as the bible of spectroscopy. In volume I he lists all the finite subgroups of the orthogonal group $O_3(\mathbb{R})$ of Euclidean space as possible molecular symmetry groups. The icosahedral group occurred in his list, but he added in a footnote that it is highly unlikely that this group will appear in nature as symmetry group. The experimental discovery in 1985 of C_{60} with its rich icosahedral symmetry came therefore as a big surprise. For this work Curl, Kroto and Smalley were awarded the Nobel prize for Chemistry in 1996. For their discovery of the flat analogue of the bucky ball, the so called graphene molecule, Andre Geim and Konstantin Novoselov were awarded the Nobel prize for Physics in 2010. Earlier that year Andre Geim was appointed honorary professor at the Radboud University Nijmegen, helping our university to win its first Nobel prize.

5 The spin homomorphism

Since for $z_1, z_2, w_1, w_2 \in \mathbb{C}$

$$\begin{pmatrix} z_1 & w_1 \\ -\bar{w}_1 & \bar{z}_1 \end{pmatrix} \begin{pmatrix} z_2 & w_2 \\ -\bar{w}_2 & \bar{z}_2 \end{pmatrix} = \begin{pmatrix} z_1 z_2 - w_1 \bar{w}_2 & z_1 w_2 + w_1 \bar{z}_2 \\ -\bar{w}_1 z_2 - \bar{z}_1 \bar{w}_2 & -\bar{w}_1 w_2 + \bar{z}_1 \bar{z}_2 \end{pmatrix}$$

it follows that

$$\mathbb{H} = \left\{ \begin{pmatrix} z & w \\ -\bar{w} & \bar{z} \end{pmatrix}; z, w \in \mathbb{C} \right\}$$

is an associative algebra over \mathbb{R} of dimension 4, called the *quaternion* algebra. They were introduced by William Hamilton (1805-1865) on Monday 16 October 1843, who carved their multiplication rule

$$i^2 = j^2 = k^2 = ijk = -1$$

for the real basis

$$1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, i = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, j = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, k = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.$$

into a stone of Brougham Bridge over the Royal Canal in Dublin, as he paused on it. We shall write quaternions as

$$q = z + wj = u_0 + u_1i + u_2j + u_3k$$

with $z = u_0 + u_1i, w = u_2 + u_3i \in \mathbb{C}$ and $u_0, u_1, u_2, u_3 \in \mathbb{R}$. We denote by $\bar{q} = u_0 - u_1i - u_2j - u_3k$ the *conjugate* quaternion of q . The *norm* $|q| = \sqrt{\det q} = \sqrt{q\bar{q}}$ is a multiplicative map from \mathbb{H} to $\mathbb{R}_{\geq 0}$, turning \mathbb{H} into an associative *division algebra*. This means that every nonzero quaternion q has an inverse, indeed namely $\bar{q}/|q|^2$. We shall denote $\Re q = u_0 \in \mathbb{R}$ for the *real part* and $\Im q = u_1i + u_2j + u_3k \in \mathbb{R}^3$ for the *imaginary part* of $q \in \mathbb{H}$. A quaternion q is called *real* if $q = \Re q$ and *purely imaginary* if $q = \Im q$.

The norm 1 quaternions form a group denoted $\mathrm{SU}_2(\mathbb{C}) \cong \mathrm{U}_1(\mathbb{H})$ just like the norm 1 complex numbers form a group denoted $\mathrm{SO}_2(\mathbb{R}) \cong \mathrm{U}_1(\mathbb{C})$. Both $\mathrm{SU}_2(\mathbb{C})$ and $\mathrm{SO}_2(\mathbb{R})$ are smooth manifolds, the latter the unit circle and the former the unit sphere of dimension 3. The multiplication and inversion on $\mathrm{SU}_2(\mathbb{C})$ and $\mathrm{SO}_2(\mathbb{R})$ is given by smooth maps and as such these are primary examples of compact Lie groups.

Let $\text{SO}_3(\mathbb{R})$ be the special orthogonal group of the Euclidean space \mathbb{R}^3 . In the sequel we shall identify \mathbb{R}^3 with the subspace of purely imaginary quaternions in \mathbb{H} . The map

$$\pi : \text{SU}_2(\mathbb{C}) \rightarrow \text{GL}_3(\mathbb{R}), \pi(q)(u) = qu\bar{q}$$

for $q \in \text{SU}_2(\mathbb{C})$ and $u \in \mathbb{R}^3$ is called the *spin homomorphism*.

Theorem 5.1. *The spin homomorphism $\pi : \text{SU}_2(\mathbb{C}) \rightarrow \text{SO}_3(\mathbb{R})$ has image $\text{SO}_3(\mathbb{R})$ and kernel ± 1 .*

Proof. For $q \in \mathbb{H}$ we have $q \in \text{SU}_2(\mathbb{C})$ if and only if $\bar{q} = q^{-1}$ which in turn implies that $\pi : \text{SU}_2(\mathbb{C}) \rightarrow \text{GL}_3(\mathbb{R})$ is a homomorphism. In order to see that the image of π is contained in $\text{SO}_3(\mathbb{R})$ we use the formula

$$uv = (u, v) + u \times v$$

for $u, v \in \mathbb{R}^3$ expressing the multiplication of purely imaginary quaternions in terms of the scalar product (\cdot, \cdot) and vector product $\cdot \times \cdot$ on \mathbb{R}^3 . It follows that

$$(\pi(q)u, \pi(q)v) = (u, v), (\pi(q)u) \times (\pi(q)v) = \pi(q)(u \times v)$$

for all $u, v \in \mathbb{R}^3$ and therefore $\pi(q) \in \text{SO}_3(\mathbb{R})$ for all $q \in \text{SU}_2(\mathbb{C})$.

Since the center of \mathbb{H} is equal to \mathbb{R} it follows that $q \in \text{SU}_2(\mathbb{C})$ commutes with all purely imaginary quaternions if and only if $q = \pm 1$.

It remains to check that the image of π equals $\text{SO}_3(\mathbb{R})$. It is known (and due to Leonard Euler (1707-1783) in his work on rigid body motions) that each element r of $\text{SO}_3(\mathbb{R})$ is a rotation around a directed axis $\mathbb{R}w$ for some unit vector $w \in \mathbb{R}^3$ over an angle $\theta \in \mathbb{R}/2\pi\mathbb{Z}$. In other words, such a rotation r is given by

$$ru = u \cos \theta + v \sin \theta, rv = -u \sin \theta + v \cos \theta, rw = w$$

in an orthonormal basis $\{u, v, w\}$ of \mathbb{R}^3 with $u \times v = w$. The straightforward verification that the unit quaternion $q = \cos \theta + w \sin \theta$ satisfies $\pi(q) = r$ is left to the reader. Hence the theorem follows. \square

By the homomorphism theorem it follows that $\text{SU}_2(\mathbb{C})/\{\pm 1\} \cong \text{SO}_3(\mathbb{R})$. Geometrically the group $\text{SU}_2(\mathbb{C})$ is the unit sphere S^3 of dimension 3. The spin homomorphism identifies antipodal points and so geometrically $\text{SO}_3(\mathbb{R})$

is just the real projective space $\mathbb{P}^3(\mathbb{R})$ of dimension 3. The orthogonal projection map

$$\mathfrak{R} : \mathrm{SU}_2(\mathbb{C}) \rightarrow [-1, 1]$$

is a class function on $\mathrm{SU}_2(\mathbb{C})$ and the conjugation classes are in fact the level surfaces of this map. The two conjugation classes $\mathfrak{R}^{-1}(\pm 1) = \pm 1$ are just points and the remaining classes are spheres of dimension 2. Hence the circle subgroup $\mathbb{R}/2\pi\mathbb{Z} \cong \mathrm{U}_1(\mathbb{C})$ of $\mathrm{SU}_2(\mathbb{C}) \cong \mathrm{U}_1(\mathbb{H})$ intersects each conjugation class in at most 2 points, which are inverses of each other.

Lemma 5.2. *If μ_E is the Euclidean measure on the unit sphere S^3 in \mathbb{H} then for each class function $\phi \in \mathrm{C}(\mathrm{SU}_2(\mathbb{C}))$ we have the integral formula*

$$\int_{S^3} \phi(x) d\mu_E(x) = 2\pi \int_0^{2\pi} \phi(\cos \theta + i \sin \theta) \sin^2 \theta d\theta$$

and so the Euclidean volume of S^3 is equal to $2\pi^2$.

Proof. For $0 < \theta < \pi$ the conjugation class of the element $(\cos \theta + i \sin \theta)$ in $\mathrm{SU}_2(\mathbb{C})$ is a sphere of dimension 2 with radius $\sin \theta$ and so with Euclidean area $4\pi \sin^2 \theta$. Since class functions on $\mathrm{SU}_2(\mathbb{C})$ restrict to even functions on $\mathrm{U}_1(\mathbb{C}) \cong \mathbb{R}/2\pi\mathbb{Z}$ the integral formula follows from calculus. The Euclidean volume of S^3 follows from this integral formula by taking $\phi = 1$. \square

Corollary 5.3. *If μ is the normalized invariant measure on $\mathrm{SU}_2(\mathbb{C})$ then*

$$\int_{\mathrm{SU}_2(\mathbb{C})} \phi(x) d\mu(x) = \frac{1}{4\pi} \int_0^{2\pi} \phi(\cos \theta + i \sin \theta) \Delta(\theta) \overline{\Delta(\theta)} d\theta$$

with $\phi \in \mathrm{C}(\mathrm{SU}_2(\mathbb{C}))$ a class function on $\mathrm{SU}_2(\mathbb{C})$ and $\Delta(\theta) = (e^{i\theta} - e^{-i\theta})$ an odd integral Fourier polynomial on $\mathrm{U}_1(\mathbb{C}) \cong \mathbb{R}/2\pi\mathbb{Z}$.

Theorem 5.4. *The restriction of the irreducible characters of $\mathrm{SU}_2(\mathbb{C})$ to $\mathrm{U}_1(\mathbb{C})$ are of the form*

$$\chi_n(\cos \theta + i \sin \theta) = \frac{e^{i(n+1)\theta} - e^{-i(n+1)\theta}}{e^{i\theta} - e^{-i\theta}} = \frac{\sin(n+1)\theta}{\sin \theta}$$

for some $n \in \mathbb{N} = \{0, 1, 2, \dots\}$.

Proof. Let (ρ, V) be an irreducible representation of $SU_2(\mathbb{C})$ with irreducible character $\chi = \text{tr } \rho$ a class function on $SU_2(\mathbb{C})$. The irreducible representations of the circle group $U_1(\mathbb{C}) \cong \mathbb{R}/2\pi\mathbb{Z}$ were shown to be of the form $\rho_n(e^{i\theta}) = e^{in\theta}$ for some $n \in \mathbb{Z}$. The restriction $\chi(\cos \theta + i \sin \theta)$ of χ to $U_1(\mathbb{C})$ is an even integral Fourier polynomial, and so the function $\chi(\cos \theta + i \sin \theta)\Delta(\theta)$ is an odd integral Fourier polynomial. Note that the Fourier coefficients of the $\chi(\cos \theta + i \sin \theta)$ are all ≥ 0 .

Taking $\phi = \chi\bar{\chi}$ in the integral formula of the above corollary yields

$$\frac{1}{2\pi} \int_0^{2\pi} \chi(\cos \theta + i \sin \theta)\Delta(\theta)\overline{\chi(\cos \theta + i \sin \theta)\Delta(\theta)}d\theta = 2$$

by the Schur orthogonality relation $\langle \chi, \chi \rangle = 1$. Writing

$$\chi(\cos \theta + i \sin \theta)\Delta(\theta) = \sum a_n e^{in\theta}$$

this amounts to $\sum a_n \bar{a}_n = 2$ and since $a_{-n} = -a_n$ also to $\sum_{n>0} a_n \bar{a}_n = 1$. By integrality of a_n we conclude that all a_n for $n > 0$ are equal to 0 with the exception of one, which is equal to ± 1 . In other words, we have

$$\chi_n(\cos \theta + i \sin \theta)\Delta(\theta) = \pm(e^{i(n+1)\theta} - e^{-i(n+1)\theta})$$

for some $n \geq 0$. Since all Fourier coefficients of $\chi_n(\cos \theta + i \sin \theta)$ are ≥ 0 the \pm becomes $+$ and the theorem follows. \square

The irreducible representation (ρ_n, V_n) of $SU_2(\mathbb{C})$ with the irreducible character χ_n as in the theorem has dimension $\chi_n(1) = (n+1)$ by l' Hopital's rule. If we denote by ρ the standard representation of $SU_2(\mathbb{C})$ on \mathbb{C}^2 then it is easy to check that the representation $\rho_n = S^n \rho$ on the space $V_n = S^n V$ of binary forms of degree n has character equal to

$$\chi_n(\cos \theta + i \sin \theta) = e^{in\theta} + e^{i(n-2)\theta} + \dots + e^{-i(n-2)\theta} + e^{-in\theta}$$

and coincides with the character found in the above theorem. The conclusion is that the degree n binary forms representation of $SU_2(\mathbb{C})$ is irreducible and in fact these are all the irreducible representations of $SU_2(\mathbb{C})$ up to equivalence.

Remark 5.5. *Mathematicians parametrize the irreducible representations of $SU_2(\mathbb{C})$ by the degree $n \in \mathbb{N}$ of the binary forms. However, physicists*

sometimes use the spin $l = \frac{1}{2}n \in \frac{1}{2}\mathbb{N}$ instead. Since $\rho_n(-1) = (-1)^n$ the irreducible representation ρ_n descends to the rotation group $\mathrm{SO}_3(\mathbb{R})$ in case the degree n is even or equivalently the spin $l = \frac{1}{2}n$ is integral. The irreducible representations with half integral spin are no longer honest representations of the rotation group $\mathrm{SO}_3(\mathbb{R})$ but only of the double spin cover $\mathrm{SU}_2(\mathbb{C})$.

The group $\mathrm{SU}_2(\mathbb{C})$ is the simplest (nontrivial) example of a connected simply connected compact Lie group. The method of this section has been generalized by Hermann Weyl (1885-1955) in 1925 to any connected simply connected compact Lie group G . One chooses a maximal torus $T \cong \mathbb{R}^n/2\pi L$ in G with L a lattice in \mathbb{R}^n . It can be shown that any two maximal tori in G are conjugated, which in turn implies that the dimension n of T is an invariant of G , called the rank of G . The rank of $\mathrm{SU}_2(\mathbb{C})$ is one and in fact $\mathrm{SU}_2(\mathbb{C})$ is the only connected simply connected compact Lie group of rank one.

The character χ of an irreducible representation of G is now completely determined by its restriction $\chi|_T$ to the torus T . By representation theory of T and structure theory of G it follows that $\chi|_T$ is an integral Fourier polynomial on T , which is invariant under the Weyl group $W = N/T$ with $N = \{x \in G; xtx^{-1} \in T \forall t \in T\}$ the normalizer of T in G . The Weyl group W acts on T by conjugation as a finite group generated by reflections. Weyl group invariant Fourier polynomials on T are just even Fourier polynomials on the circle group $\mathbb{R}/2\pi\mathbb{Z}$ in the $\mathrm{SU}_2(\mathbb{C})$ case.

The irreducibility criterion $\langle \chi, \chi \rangle = 1$ can be used along the same lines as above for $\mathrm{SU}_2(\mathbb{C})$ to write $\chi|_T$ as the quotient of two alternating integral Fourier polynomials on T . This is the famous Weyl character formula, and is considered one of the highlights of Weyl's work. Weyl's approach is transcendental using integration theory. A purely algebraic approach to Weyl's character formula was found by the German-Dutch mathematician Hans Freudenthal (1905-1990) in 1954.

The original approach of Weyl is explained for example in the text book J.J. Duistermaat and J.A.C. Kolk, Lie groups, Springer, 1999. The text book H. Freudenthal and H. de Vries, Linear Lie Groups, Academic Press, 1969 was the first modern exposition of the subject, and explains both approaches. It has interesting historical comments. Unfortunately, the notation is quite unusual, probably due to certain ideas of Freudenthal on the didactics of mathematics. This is also probably the main reason that the book did not have the influence, which it deserved. Henk de Vries was my former colleague

here in Nijmegen. Hans Duistermaat, one of my two PhD advisors, was PhD student and successor of Hans Freudenthal in Utrecht. The mathematical institute in Utrecht is located in the Freudenthal building, named in 2013 after Freudenthal, to commemorate his contributions for Dutch mathematics.

Exercise 5.1. *Show Euler's result that each element $r \in \text{SO}_3(\mathbb{R})$ is a rotation around some axis over some angle, and so of the form*

$$ru = u \cos \theta + v \sin \theta, rv = -u \sin \theta + v \cos \theta, rw = w$$

for some orthonormal basis $\{u, v, w\}$ of \mathbb{R}^3 with $u \times v = w$.

Exercise 5.2. *The group $\text{SO}_4(\mathbb{R})$ is the connected group of isometries of the sphere $S^3 \cong \text{SU}_2(\mathbb{C})$. Show that there exists a spin double cover homomorphism $\text{SU}_2(\mathbb{C}) \times \text{SU}_2(\mathbb{C}) \rightarrow \text{SO}_4(\mathbb{R})$ with kernel $\{\pm(-1, -1)\}$ of order 2.*

Exercise 5.3. *Show using character theory the Clebsch-Gordan rule*

$$\rho_n \otimes \rho_m \sim \rho_{n+m} \oplus \rho_{n+m-2} \oplus \cdots \oplus \rho_{|n-m|+2} \oplus \rho_{|n-m|}$$

for the decomposition of the tensor product of two irreducible representations of $\text{SU}_2(\mathbb{C})$ as direct sum of irreducible representations.

6 Lie groups

For M a smooth manifold let us denote by $\mathfrak{X}(M)$ the linear space of smooth vector fields on M . Let us denote for $X \in \mathfrak{X}(M)$ by \mathcal{L}_X the derivative in the direction of X acting on $C^\infty(M)$. The linear operator $\mathcal{L}_X : C^\infty(M) \rightarrow C^\infty(M)$ is a derivation of the commutative algebra $C^\infty(M)$ in the sense that $\mathcal{L}_X(\phi\psi) = \mathcal{L}_X(\phi)\psi + \phi\mathcal{L}_X(\psi)$ for all $\phi, \psi \in C^\infty(M)$. Conversely any linear derivation on $C^\infty(M)$ is of the form \mathcal{L}_X for some $X \in \mathfrak{X}(M)$. It turns out that the map

$$\mathfrak{X}(M) \rightarrow \text{Der}(C^\infty(M)), X \mapsto \mathcal{L}_X$$

is a linear bijection. Here we denote by $\text{Der}(A)$ the linear subspace of $\text{End}(A)$ of all derivations of an associative algebra A . For $D_1, D_2 \in \text{Der}(A)$ it is easy to check that the commutator bracket $[D_1, D_2] = D_1D_2 - D_2D_1$ in $\text{End}(A)$ is again a derivation, and so $\text{Der}(A)$ is closed under brackets. In turn it follows easily that

$$[[D_1, D_2], D_3] + [[D_2, D_3], D_1] + [[D_3, D_1], D_2] = 0$$

for all $D_1, D_2, D_3 \in \text{Der}(A)$, which is called the *Jacobi identity*.

A *Lie group* G is both a group and a smooth manifold, and the two structures of group and manifold are compatible in the sense that the multiplication $G \times G \rightarrow G$ and inversion $G \rightarrow G$ are smooth maps. They are named after the Norwegian mathematician Sophus Lie (1842-1899) who initiated the study of smooth symmetry and applied this to questions of geometry and differential equations.

The smooth map $l_x : G \rightarrow G, y \mapsto xy$ of left multiplication by $x \in G$ is a bijection with inverse $l_{x^{-1}}$. Its tangent map

$$T_y l_x : T_y G \rightarrow T_{xy} G$$

at $y \in G$ is a linear isomorphism with inverse $T_{xy} l_{x^{-1}}$. A smooth vector field $X \in \mathfrak{X}(G)$ on G is called *left invariant* if $T_y l_x$ maps X_y to X_{xy} for all $x, y \in G$. Let us denote for $X \in \mathfrak{X}(G)$ by \mathcal{L}_X the directional or Lie derivative acting on $C^\infty(G)$. The left regular representation of G on $C^\infty(G)$ is defined by $(\lambda(x)\phi)(y) = \phi(x^{-1}y)$ just as for finite groups. Then $X \in \mathfrak{X}(G)$ is left invariant if and only $\mathcal{L}_X \lambda(x) = \lambda(x)\mathcal{L}_X$ for all $x \in G$.