Representations of groups

Linear spaces (often also called vector spaces)

We shall consider vector spaces over the field of real or complex numbers. A linear space $\mathcal{V}$ is a non-empty set of elements (called vectors) $\mathbf{v}$ that obey the following axioms:

- A binary operation (vector addition) is defined:
  $\forall \mathbf{v}_1, \mathbf{v}_2 \in \mathcal{V} \; \exists! \mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2 \in \mathcal{V}$;
- A binary function (scalar multiplication) is defined:
  $\forall$ number c and $\forall \mathbf{v} \in \mathcal{V} \; \exists! \mathbf{u} = c\mathbf{v} \in \mathcal{V}$;
- Associativity: $\mathbf{v}_1 + (\mathbf{v}_2 + \mathbf{v}_3) = (\mathbf{v}_1 + \mathbf{v}_2) + \mathbf{v}_3$;
- Commutativity: $\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{v}_2 + \mathbf{v}_1$;
- Identity element of vector addition:
  $\exists \mathbf{0} \in \mathcal{V} : \; \forall \mathbf{v} \in \mathcal{V} \;\; \mathbf{0} + \mathbf{v} = \mathbf{v}$;
- Inverse elements of vector addition:
  $\forall \mathbf{v} \in \mathcal{V} \; \exists (-\mathbf{v}) \in \mathcal{V} : \; \mathbf{v} + (-\mathbf{v}) = \mathbf{0}$;

Axioms (continued)

- Compatibility of scalar-to-scalar multiplication with scalar-to-vector multiplication: $(c_1 c_2)\mathbf{v} = c_1(c_2\mathbf{v})$;
- Multiplication by unity: $1\,\mathbf{v} = \mathbf{v}$;
- Distributivity of scalar multiplication with respect to vector addition: $c(\mathbf{v}_1 + \mathbf{v}_2) = c\mathbf{v}_1 + c\mathbf{v}_2$;
- Distributivity of scalar multiplication with respect to addition of scalars: $(c_1 + c_2)\mathbf{v} = c_1\mathbf{v} + c_2\mathbf{v}$.

Recalling the main concepts

- Linear combination;
- Linear independence;
- Linear subspace;
- Linear span of a subset;
- Basis and dimension.

Linear operators

$$\hat{T} : \mathcal{V} \mapsto \mathcal{V}$$

For all vectors and numbers

$$\hat{T}(c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2) = c_1 \hat{T} \mathbf{v}_1 + c_2 \hat{T} \mathbf{v}_2$$

Identity operator $\hat{E}$:

$$\forall \mathrm{v} \in \mathcal{V} \qquad \hat{E}\mathrm{v} = \mathrm{v}$$

Representation of a group: Definition

A representation T of a group G is defined if each $g \in G$ corresponds to a certain linear operator $\hat{T}(g)$ in a certain linear space $\mathcal{L}$ such that

$$\hat{T}(g_1 g_2) = \hat{T}(g_1)\hat{T}(g_2)$$

Homomorphism between G and the group of operators.

dim $\mathcal{L}$ is called the dimension of the representation.
dim $\mathcal{L}$ may be infinite; we focus on representations of finite dimension.

Special case: Unit representation

$\forall g \in G : \hat{T}(g) = \hat{E}$ in a certain $\mathcal{L}$.

This representation is called the unit representation.

It is sufficient to have $\dim \mathcal{L} = 1$.

Schrödinger equations and its symmetry group

Consider, for the sake of simplicity, the single-particle Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + U(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

The operator $-\nabla^2$ is invariant under inversion and all 3D rotations and translations.
The potential $U(\mathbf{r})$ may remain invariant under a certain group G (point group or periodic translations).

$$\forall g \in G: \ \hat{T}(g)f(\mathbf{r}) = f(g\mathbf{r}).$$

By assumption, $U(g\mathbf{r}) = U(\mathbf{r})$.
We apply $\hat{T}(g)$ to both sides of the Schrödinger eq. and obtain

$$-\frac{\hbar^2}{2m}\nabla^2\psi(g\mathbf{r}) + U(\mathbf{r})\psi(g\mathbf{r}) = E\psi(g\mathbf{r}).$$

Obviously, $\hat{T}(g_1)\hat{T}(g_2) = \hat{T}(g_1 g_2)$.

The number of linearly independent functions $\psi(g\mathbf{r})$, where we take all elements $g \in G$, is the dimension of the linear space $\mathcal{L}$, where a representation T is defined.

Functional of averaging

$$\varphi: \ G \mapsto \mathbb{R} \quad \text{or} \quad G \mapsto \mathbb{C}$$

I.e., for each $g \in G$ a real (or complex) number $\varphi(g)$ is defined.
For a finite group G of the order N:

$$M(\varphi) = \frac{1}{N} \sum_{g \in G} \varphi(g)$$

1. $\forall g \in G: \ \varphi(g) > 0 \ \Rightarrow \ M(\varphi) > 0$
2. $\forall g \in G: \ \varphi(g) = 1 \ \Rightarrow \ M(\varphi) = 1$
3. If $\chi(g) = \varphi(gh)$ and $\tilde{\chi}(g) = \varphi(hg)$, where $h \in G$, then

$$M(\chi) = M(\tilde{\chi}) = M(g)$$

The proof using the uniqueness of h^{-1}:

$$M(\chi) = \frac{1}{N} \sum_{g \in G} \chi(g) = \frac{1}{N} \sum_{g \in G} \varphi(gh) = \frac{1}{N} \sum_{g \in G} \varphi(g) = M(g)$$

An extension to some (not all!) infinite groups is possible.
E.g., for the rotation group (Euler angles α, β, γ):

$$M(\varphi) = \frac{1}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \, \sin\beta \int_0^{2\pi} d\gamma \, \varphi(\alpha, \beta, \gamma)$$

Or, recalling Wigner D-functions for half-integer spins,

$$M(\varphi) = \frac{1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \, \sin\beta \int_0^{2\pi} d\gamma \, \varphi(\alpha, \beta, \gamma)$$

Equivalent representations

Assume that T is a representation of G in $\mathcal{L}$.
A non-singular operator $\hat{A}$: $\mathcal{L} \mapsto \mathcal{L}_1$, $\quad \dim \mathcal{L}_1 = \dim \mathcal{L}$.

$$\hat{T}_A(g) = \hat{A}\hat{T}(g)\hat{A}^{-1}$$

$g \mapsto \hat{T}_A(g)$ is an equivalent representation in $\mathcal{L}_1$.

$$\hat{T}_A(g_1 g_2) = \hat{A}\hat{T}(g_1 g_2)\hat{A}^{-1} = \hat{A}\hat{T}(g_1)\hat{T}(g_2)\hat{A}^{-1} =$$

$$\hat{A}\hat{T}(g_1)\hat{A}^{-1}\hat{A}\hat{T}(g_2)\hat{A}^{-1} = \hat{T}_A(g_1)\hat{T}_A(g_2)$$

All representations of G can be divided into classes of mutually equivalent representations. It is sufficient to know one representation from each class.

Each class of equivalent representations contains at least one unitary representation, i.e., such T that $\forall g \in G$: $[\hat{T}(g)]^\dagger = [\hat{T}(g)]^{-1}$.

Proof. Let $\langle \mathbf{u}|\mathbf{v}\rangle$ be a scalar product of vectors defined in $\mathcal{L}$. Then

$$(\mathbf{u}|\mathbf{v}) = \frac{1}{N}\sum_{h\in G}\langle \mathbf{u}|[\hat{T}(h)]^{\dagger}\hat{T}(h)|\mathbf{v}\rangle$$

satisfies all the requirements for a scalar product, namely,

$$(\mathbf{u}|a_1\mathbf{v}_1 + a_2\mathbf{v}_2) = a_1(\mathbf{u}|\mathbf{v}_1) + a_2(\mathbf{u}|\mathbf{v}_2),$$

$$(\mathbf{v}|\mathbf{v}) > 0, \quad \mathbf{v} \neq \mathbf{0}$$

(the latter inequality follows from the 1st property of the averaging functional).

$$(\mathbf{u}|[\hat{T}(g)]^{\dagger}\hat{T}(g)|\mathbf{v}) = \frac{1}{N}\sum_{h\in G}\langle \mathbf{u}|[\hat{T}(h)]^{\dagger}[\hat{T}(g)]^{\dagger}\hat{T}(g)\hat{T}(h)|\mathbf{v}\rangle =$$

$$= \frac{1}{N}\sum_{h\in G}\langle \mathbf{u}|[\hat{T}(gh)]^{\dagger}\hat{T}(gh)|\mathbf{v}\rangle = \frac{1}{N}\sum_{h\in G}\langle \mathbf{u}|[\hat{T}(h)]^{\dagger}\hat{T}(h)|\mathbf{v}\rangle = (\mathbf{u}|\mathbf{v})$$

Operators $\hat{T}(g)$ are unitary w. resp. to $(\ldots|\ldots)$.

Knowing a certain representation T, we can construct an equivalent unitary representation.

$\dim \mathcal{L} = s$

"Old" basis: $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_s\}, \quad \langle \mathbf{e}_i | \mathbf{e}_k \rangle = \delta_{ik}$

"New" basis: $\{\mathbf{e}'_1, \mathbf{e}'_2, \ldots, \mathbf{e}'_s\}, \quad (\mathbf{e}'_i | \mathbf{e}'_k) = \delta_{ik}$

Define an operator $\hat{A}$ such that $\hat{A}\mathbf{e}_i = \mathbf{e}'_i, \quad i = 1, 2, \ldots, s.$ Then the representation

$$\hat{T}_A(g) = \hat{A}^{-1}\hat{T}(g)\hat{A}$$

possesses the unitarity property,

$$(\mathbf{u}|[\hat{T}_A(g)]^\dagger \hat{T}_A(g)|\mathbf{v}) = (\mathbf{u}|\mathbf{v})$$