Notes for B7—Symmetry

A pedantic summary of important points

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Some of the more mathematical issues in this course are rather hard to condense and verbalise in the supervisions. I have therefore compiled this set of notes to go over these issues more carefully. I hope that this will provide a more satisfactory and rigorous account of the group and representation theory encountered in this course. The main purpose of these notes is to enhance your understanding and help you become more familiar and comfortable with the mathematical arguments and techniques involved in group and representation theory. Some of the concepts mentioned here will definitely not be required for the Tripos examination of this course, so please do not feel compelled to remember all of them. A good read of these notes in conjunction with the main lecture handout and a thorough revision of the supervision questions will place you in a very good position to understand the key points of the course and the significance of symmetry in illuminating the quantum world.

1 Preliminaries

We introduce several mathematical preliminaries in this Section to prepare for a more rigorous treatment in what will follow.

1.1 Maps

Maps enable objects from different sets or collections to be associated with one another. In our study of groups and their representations, we will very often have to relate elements of various different groups together. A clear understanding of maps allows us to think about group relationships more logically.

Definition 1.1.1 (Map). Let X and Y be sets. A *map* $f : X \to Y$ is a rule that associates to each element $x \in X$ a unique element $f(x) \in Y$. We can then write $f : x \mapsto f(x)$. X and Y are called the *domain* and the *target* of the map f, respectively.

Example 1.1.1.

(a) The map $f : \mathbb{R} \to \mathbb{C}$ defined by $f : x \mapsto x + ix$ sends each real number x to a unique complex number $x + ix$.

(b) The map $f : \mathbb{R} \times \mathbb{R} \to \mathbb{C}$ defined by $f : (x, y) \mapsto x + iy$ sends each ordered pair of real numbers (x, y) to a unique complex number $x + iy$.

Definition 1.1.2 (Injective map). A map $f : X \to Y$ is *injective* if it sends unique elements of X to unique elements of Y. This means that, for all $x, x' \in X$, $x \neq x' \implies f(x) \neq f(x')$, or equivalently, $f(x) = f(x') \implies x = x'$.

Definition 1.1.3 (Surjective map). A map $f : X \to Y$ is *surjective* if, for each $y \in Y$, there is some $x \in X$ such that $f(x) = y$.

Example 1.1.2.

(a) The map $f : \mathbb{R} \to \mathbb{C}$ with $x \mapsto x + ix$ is injective because $x + ix = x' + ix' \implies x = x'$. However, it is not surjective because there is no $x \in \mathbb{R}$ that gets mapped to $(1 + 2i) \in \mathbb{C}$.

(b) The map $f : \mathbb{R} \to \mathbb{R}_0^+$ with $x \mapsto x^2$ is not injective because $-2 \neq 2$ but $(-2)^2 = 2^2 = 4$. However, it is surjective because every non-negative real number $y \in \mathbb{R}_0^+$ must be the square of some real number.

Definition 1.1.4 (Bijective map)**.** A map $f : X \to Y$ is *bijective* if it is both surjective and injective, *i.e.*, f sends every $x \in X$ to one and only one $y \in Y$, and every $y \in Y$ has exactly one $x \in X$ that gets sent to it.

Example 1.1.3. The map $f : \mathbb{R} \to \mathbb{R}$ with $x \mapsto 5x + 2$ is bijective.

Definition 1.1.5 (Image)**.** Consider a map $f : X \to Y$. The set $\{y \in Y : y = f(x) \text{ for all } x \in X\}$ is a subset of Y called the *image* of f. We denote this set $\operatorname{im} f$ (the green area in Figure 1).

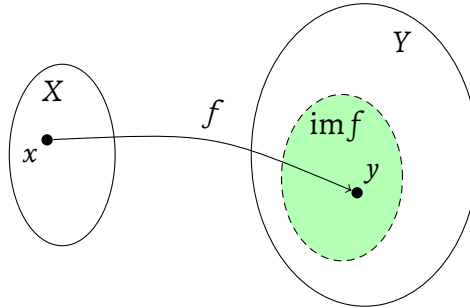Combining this Definition with Definition 1.1.3, we see that f is surjective if and only if $\operatorname{im} f = Y$.

Figure 1: Image of the map $f : X \to Y$.

Example 1.1.4. The image of the map $f : \mathbb{R} \to \mathbb{R}$ with $x \mapsto x^2$ is $\operatorname{im} f = \mathbb{R}_0^+$. Clearly $\mathbb{R}_0^+ \subset \mathbb{R}$ and f is not surjective. But if we restrict the target of f to $\mathbb{R}_0^+$, then, as in Example 1.1.2(b), f is surjective.

1.2 Groups

You should be very familiar with all of the following definitions. However, they are included here, together with a few interesting examples, for completeness.

Definition 1.2.1 (Binary operation)**.** A *binary operation* on a set X is a map $\star : X \times X \to X$ that combines two elements in X to give another element in X.

Definition 1.2.2 (Group). A *group* is a triple $(G, \star, e)$ of a set G, a binary operation $\star$ on G, and an element $e \in G$ such that

   (i) (closure) for all $a, b \in G$, $a \star b \in G$;

   (ii) (associativity) for all $a, b, c \in G$, $(a \star b) \star c = a \star (b \star c)$;

  (iii) (identity) for all $a \in G$, $a \star e = e \star a = a$;

  (iv) (inverse) for all $a \in G$, there exists some $b \in G$ such that $a \star b = b \star a = e$.

Remark. We will write G to denote the group $(G, \star, e)$ whenever the binary operation $\star$ and the identity element e is clear from context.

Definition 1.2.3 (Abelian group). A group $(G, \star, e)$ is called *abelian* if $a \star b = b \star a$ for all $a, b \in G$.

Example 1.2.1. The point groups $\mathcal{C}_{2v}$, $\mathcal{D}_{2h}$, and all cyclic groups (*e.g.*, $\mathcal{C}_3$) are some notable abelian groups.

Definition 1.2.4 (Group presentation). A *presentation* of a group $(G, \star, e)$, denoted by $\langle S \mid R \rangle$, consists of a set S of *generators* and a set R of *relations* amongst these generators. Every element in G can be written as a product of powers of some of these generators, with respect to the binary operation $\star$.

Example 1.2.2.

  (a) The cyclic group $\mathcal{C}_n$ has presentation $\langle r \mid r^n = e \rangle$. In point-group symmetry, we identify r with an n-fold rotation about some axis C_n.

  (b) The dihedral groups $\mathcal{D}_{nh}$ has presentation $\langle r, s, t \mid r^n = s^2 = t^2 = e \rangle$. In point-group symmetry, we identify r with an n-fold rotation about some axis C_n, s a two-fold rotation about an axis $C_2 \perp C_n$, and t a reflection in a plane $\sigma_h \perp C_n$.

Definition 1.2.5 (Group finiteness and order). A group $(G, \star, e)$ is called *finite* if it has a finite number of elements. Otherwise, it is called *infinite*. We write $|G|$ (or commonly h in Physics and Chemistry) for the number of elements of G and call this the *order* of the group.

Example 1.2.3.

  (a) The cyclic group $\mathcal{C}_n = (\langle r \mid r^n = e \rangle, \star, e)$ has order n and is finite if h is finite.

(b) There is, up to isomorphism (see Definition 1.3.2), only one unique group of order 3, namely the cyclic group $\mathcal{C}_3$.

(c) There are, up to isomorphism, only two groups of order 4, namely the cyclic group $\mathcal{C}_4$ and Klein four-group. Klein four-group is isomorphic to the more familiar point groups $\mathcal{C}_{2v}$, $\mathcal{C}_{2h}$, and $\mathcal{D}_2$.

(d) $\mathcal{C}_{\infty v}$ and $\mathcal{D}_{\infty h}$ are two infinite axial point groups most commonly encountered in Chemistry.

(e) The group of all rotations in three dimensions, denoted SO(3), is an infinite group. The group of all reflections and rotations in three dimensions, denoted O(3), is also an infinite group.

1.3 Group Homomorphisms

Group homomorphisms are structure-preserving maps that relate elements from different groups to each other. These play a central role in the study of group and representation theory.

Definition 1.3.1 (Group homomorphism)**.** Let $(G, \star_G, e_G)$ and $(H, \star_H, e_H)$ be groups. A map $\varphi : G \to H$ is called a *group homomorphism* if, for all $a, b \in G$,

$$\varphi(a \star_G b) = \varphi(a) \star_H \varphi(b).$$

Remark. φ is essentially a map sending elements in one group, say, G, to elements in another group, say, H. This map is, however, slightly more special because it preserves the structure of the domain group. In particular,

(i) it preserves closure: for all $a, b \in G$,

$$\varphi(a) \star_H \varphi(b) = \varphi(a \star_G b) \in \operatorname{im} \varphi \text{ because } a \star_G b \in G,$$

i.e., the product $\varphi(a) \star_H \varphi(b)$ stays in the image of the map φ;

(ii) it preserves associativity: for all $a, b, c \in G$,

$$
\begin{aligned}
[\varphi(a) \star_H \varphi(b)] \star_H \varphi(c) &= [\varphi(a \star_G b)] \star_H \varphi(c) \\
&= \varphi[(a \star_G b) \star_G c] \\
&= \varphi[a \star_G (b \star_G c)] \\
&= \varphi(a) \star_H [\varphi(b \star_G c)] \\
&= \varphi(a) \star_H [\varphi(b) \star_H \varphi(c)];
\end{aligned}
$$

(iii) it maps the identity in G to the identity in H: for all $a \in G$,

$$
\varphi(a) = \varphi(e_G \star_G a) = \varphi(e_G) \star_H \varphi(a) \implies \varphi(e_G) = e_H;
$$

(iv) it maps inverse to inverse: for all $a \in G$,

$$
e_H = \varphi(e_G) = \varphi(a \star_G a^{-1}) = \varphi(a) \star_H \varphi(a^{-1}) \implies \varphi(a^{-1}) = \varphi(a)^{-1}.
$$

Example 1.3.1.

(a) The map $\varphi : G \to H$ defined by $\varphi : g \mapsto e_H$ is a group homomorphism. It is, however, not injective if $|G| > 1$ because different elements in G get mapped to the same element e_H in H.

(b) Let $G = (\mathbb{R}, +, 0)$ be the additive group of real numbers and $H = (\mathbb{R}^+, \times, 1)$ the multiplicative group of positive real numbers. The map $\varphi : G \to H$ defined by $\varphi : g \mapsto \exp(g)$ is a group homomorphism.

Definition 1.3.2 (Group isomorphism)**.** Let $\varphi : G \to H$ be a group homomorphism. If φ is bijective, it is called a *group isomorphism*. If there exists a group isomorphism between G and H, then G and H are said to be *isomorphic* and we write $G \cong H$.

Example 1.3.2.

(a) The map φ in Example 1.3.1(b) is bijective (why?) and is therefore an isomorphism. $(\mathbb{R}, +, 0)$ and $(\mathbb{R}^+, \times, 1)$ are therefore isomorphic.

(b) Let $\mathcal{C}_4 = \left(\langle \hat{C}_4 \mid \hat{C}_4^4 = \hat{E}\rangle, \cdot, \hat{E}\right)$ be the cyclic group of order 4 and $G = (\{1, i, -1, -i\}, \cdot, 1)$ the group generated by the imaginary unit i. The group homomorphism $\varphi : G \to \mathcal{C}_4$ given by

$$\varphi : 1 \mapsto \hat{E}, \quad i \mapsto \hat{C}_4, \quad -1 \mapsto \hat{C}_4^2, \quad -i \mapsto \hat{C}_4^3$$

is a group isomorphism. Therefore, G and $\mathcal{C}_4$ are isomorphic.

(c) The point groups $\mathcal{T}_d$ and $\mathcal{O}$ are isomorphic.

1.4 Some Important Abstract Groups

We provide a quick survey of some important abstract groups to which many of the commonly encountered concrete groups are isomorphic, and quite a few of which have far-reaching implications in quantum mechanics. The abstractness of these groups admittedly does make them quite hard to be understood at first, but having at least a notion of them helps us think about the zoo of finite and infinite groups more systematically.

1.4.1 Linear Groups

In this Section, we write $\mathbb{F}$ to denote a field that can be either $\mathbb{C}$ or $\mathbb{R}$.

Definition 1.4.1 (Vector space). Let V be an (additive) abelian group and $\mathbb{F}$ a commutative field. V is called a *vector space over* $\mathbb{F}$ if, for all elements $\boldsymbol{v}_1, \boldsymbol{v}' \in V$ and scalars $\lambda, \lambda' \in \mathbb{F}$,

(i) (distributivity) $\lambda(\boldsymbol{v} + \boldsymbol{v}') = \lambda\boldsymbol{v} + \lambda\boldsymbol{v}'$;

(ii) (distributivity) $(\lambda + \lambda')\boldsymbol{v} = \lambda\boldsymbol{v} + \lambda'\boldsymbol{v}$;

(iii) (associativity) $\lambda'(\lambda\boldsymbol{v}) = (\lambda'\lambda)\boldsymbol{v}$;

(iv) (unity) $1\boldsymbol{v} = \boldsymbol{v}$.

Remark. It is clear from the above Definition that neither a basis nor a concept of distances and angles is needed for a vector space.

We often think about V as the space of geometrical vectors in some dimensions, due mainly to its name, but V can be a much more general space than that. The following definitions of some concrete vector spaces should make this clear.

Definition 1.4.2 (Coordinate space). For a positive integer n, the set of all n-tuples of elements of $\mathbb{F}$, $\boldsymbol{v} = (x_1, x_2, \dots, x_n)$, forms an n-dimensional vector space over $\mathbb{F}$ called a *coordinate space* and denoted $\mathbb{F}^n$.

Example 1.4.1.

(a) s

(b) s

Definition 1.4.3 (Function space). Let X be a set. The set of all maps $f : X \to \mathbb{F}$ forms a vector space over $\mathbb{F}$ called a *function space* and denoted $\mathbb{F}^X$.

Proposition 1.4.1. *Let V be a vector space over a field $\mathbb{F}$. The set of all invertible linear maps $\vartheta : V \to V$ forms a group.*

Proof. This proof is left as an exercise to the reader. □

Definition 1.4.4 (General linear group). Let V be a vector space over a field $\mathbb{F}$. The group of all invertible linear maps $\vartheta : V \to V$ is called the *general linear group* of V and denoted by $\mathrm{GL}(V)$.

Remark.

(a) The binary operation in $\mathrm{GL}(V)$ is the operation of function composition, $\circ$, where $(\vartheta_2 \circ \vartheta_1)(\boldsymbol{v}) = \vartheta_2[\vartheta_1(\boldsymbol{v})]$ for some $\boldsymbol{v} \in V$.

(b) The identity of $\mathrm{GL}(V)$ is the identity map $\mathrm{id} : V \to V$ defined as $\mathrm{id} : \boldsymbol{v} \mapsto \boldsymbol{v}$ which maps each $\boldsymbol{v} \in V$ to itself.

Definition 1.4.4 does seem to make $\mathrm{GL}(V)$ look like a very abstract group. It is indeed a fairly abstract group, and it might therefore be easier to think about $\mathrm{GL}(V)$ as the group of all invertible linear transformations acting on a particular vector space and mapping each vector to another vector. Now, if V is a vector space of finite dimensions, say n, over $\mathbb{F}$, then we can choose a basis $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \dots, \boldsymbol{e}_n\}$

for V over $\mathbb{F}$ such that each vector $\boldsymbol{v} \in V$ can be written as $\boldsymbol{v} = \sum_{i=1}^{n} \boldsymbol{e}_i v_i$. Then, every invertible linear transformation $\vartheta \in GL(V)$ corresponds to an $n \times n$ invertible matrix $\boldsymbol{M}_\vartheta = [M_{ij}(\vartheta)]$ given by

$$\vartheta(\boldsymbol{e}_j) = \sum_{i=1}^{n} \boldsymbol{e}_i M_{ij}(\vartheta).$$

This motivates the following.

Proposition 1.4.2. *The set of $n \times n$ invertible matrices over $\mathbb{F}$, together with the binary operation of ordinary matrix multiplication, forms a group. We denote this group $GL_n(\mathbb{F})$.*

Proof. This proof is left as a trivial exercise to the reader. $\square$

Proposition 1.4.3. *The groups $GL(V)$ and $GL_n(\mathbb{F})$ are isomorphic with the isomorphism given by $\vartheta \mapsto \boldsymbol{M}_\vartheta$ where $\boldsymbol{M}_\vartheta$ are $n \times n$ invertible matrices.*