

- Reading: Gallian Chs. 27 & 28
- Most of the applications of group theory to the physical sciences are through the study of the symmetry groups of physical objects (e.g. molecules or crystals). Understanding the symmetries helps in understanding the objects' physical properties and in determining the structure of the objects from measurements or images.

1 Isometries

- Recall that symmetry groups of geometric objects are defined in terms of isometries, so we begin by understanding those.
- **Def:** An *isometry* of \mathbb{R}^n is a function $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that for every $x, y \in \mathbb{R}^n$, we have $\|T(x) - T(y)\| = \|x - y\|$.
 - Isometries are always permutations (bijections).
 - The set of isometries of \mathbb{R}^n forms a group under composition, known as the *Euclidean Group* E_n .
 - Isometries preserve angles: $\langle T(x), T(y) \rangle = \langle x, y \rangle$.
 - Although most physical objects live in \mathbb{R}^3 , we'll focus on objects in \mathbb{R}^2 . Symmetry of 2-D objects is useful in *surface physics*. Everything we'll discuss has generalizations to \mathbb{R}^3 .
- **Linear-algebraic Description of Isometries:**
 - **Fact:** The isometries of \mathbb{R}^n are exactly the maps of the form $T(x) = Ax + b$, where A is an $n \times n$ orthogonal matrix (i.e., $AA^t = I$, where A^t is the transpose of A) and $b \in \mathbb{R}^n$.
 - In \mathbb{R}^2 , the possible orthogonal matrices A are:

$$\text{Rot}_\theta = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}, \text{ and } \text{Ref}_\theta = \begin{pmatrix} -\cos \theta & \sin \theta \\ \sin \theta & \cos \theta \end{pmatrix},$$

for $\theta \in [0, 2\pi)$. Rot_θ is a clockwise rotation around the origin by angle θ . Ref_θ is a reflection through the axis that is the y -axis rotated clockwise by angle $\theta/2$.

- **Classification of Isometries** $T(x) = Ax + b$ of \mathbb{R}^2 :

- $A = \text{Rot}_0 = I$: T is a *translation*.

¹These notes are copied mostly verbatim from the lecture notes from the Fall 2010 offering, authored by Prof. Salil Vadhan. I will attempt to update them, but apologies if some references to old dates and contents remain.

- $A = \text{Rot}_\theta$ for $\theta \in (0, 2\pi)$: T is a clockwise *rotation* by θ degrees about the point $(I - A)^{-1}b$. ($I - A$ is invertible because A has no fixed points.)
 - $A = \text{Ref}_\theta$, b orthogonal to the axis ℓ of reflection: T is a *reflection* through the axis $\ell + b/2$.
 - $A = \text{Ref}_\theta$, b parallel to axis of reflection: T is a *glide-reflection*:
- $A = \text{Ref}_\theta$, b neither parallel nor perpendicular to axis of reflection: T is a *glide-reflection* along the axis $\ell + b'/2$, where b' is the component of b perpendicular to the axis of reflection.
- **Q:** What are the orders of each of the above elements (in the group of isometries of \mathbb{R}^2 under composition)?

2 Symmetry Groups

- **Def:** For a set F of points in \mathbb{R}^n , the *symmetry group* of F is the set $\text{Isom}(F)$ of isometries $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that $T(F) = F$, where $T(F) = \{T(x) : x \in F\}$, under composition.
- Many physical objects are not merely sets of points, but the points have different types (eg they may be different atoms). We can generalize the above definition to allow a set X of types of points (where X includes an element that represents no point being present) as follows:
- **Def:** For a function $F : \mathbb{R}^n \rightarrow X$, the *symmetry group* of F is the set $\text{Isom}(F)$ of isometries $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that $F \circ T = F$, under composition. That is the type $F(T(x))$ of point $T(x)$ equals the type $F(x)$ of point x , for all $x \in \mathbb{R}^n$.
- **Examples:** Silicon (100) Face. This is the 2-D crystal obtained by cutting a 3-D Silicon crystal along a particular face. When this is done the forces exerted on atoms near the surface changes, causing those atoms to shift slightly, reducing the symmetry and changing the physical properties (as we will see). This process is called *reconstruction*. The attached sheets show both the unreconstructed and reconstructed forms of the Si(100) face. All the circles are silicon atoms. The different colors and heights indicate different distances from the surface, so we treat these atoms as different from each other.
- **Important subgroups of $\text{Isom}(F)$:**
 - The *translation subgroup* $\text{Trans}(F)$ is the set of translations in $\text{Isom}(F)$. This is a normal subgroup of $\text{Isom}(F)$.
 - For $p \in \mathbb{R}^n$, the *point group* at p is $\text{Point}(F, p) = \text{stab}_G(p) = \{T \in G : T(p) = p\}$.
 - * Includes rotations around p and reflections through axis containing p .

- * May be different for different points p .
- From knowledge of $\text{Trans}(F)$ and $\text{Point}(F, p)$ for a point p of *highest rotational symmetry* (i.e. $\text{Point}(F, p)$ contains a rotation of the smallest angle among all points p), it is usually not much work to determine the full symmetry group $\text{Isom}(F)$. (See PS7.)
- Let's calculate these subgroups for our Si(100) examples.

3 Crystallographic Groups

- **Def:** A 2-D *crystal* is an infinite arrangement $F : \mathbb{R}^2 \rightarrow X$ of molecules or atoms whose translation subgroup is isomorphic to $\mathbb{Z} \times \mathbb{Z}$. That is, there are two linearly independent vectors $v_1, v_2 \in \mathbb{R}^2$ such that the translational symmetries of F are exactly those of the form $x \mapsto x + k_1 v_1 + k_2 v_2$ for integers k_1, k_2 .
- The points $\text{Latt}(F) = \{k_1 v_1 + k_2 v_2\}$ are a 2-dimensional *lattice*, consisting of points that are symmetric with the origin under translational symmetry. We call this the *translation lattice* of F .
- **Thm:** If $F : \mathbb{R}^2 \rightarrow X$ is a 2-D crystal and $p \in \mathbb{R}^2$, then $\text{Rot}(F, p)$ is of order 1, 2, 3, 4, or 6. Hence $\text{Rot}(F, p)$ is isomorphic to \mathbb{Z}_n or D_n for $n \in \{1, 2, 3, 4, 6\}$.

Proof: We'll show $n \leq 6$. The proof that $n \neq 5$ is similar. By translating, we can assume $p = 0$. Let v be a shortest nonzero vector in the translation lattice for F , and T_v be the corresponding translation. If $\text{Rot}_\theta \in \text{Point}(F, 0)$, then

$$\text{Rot}_\theta \circ T_v \circ \text{Rot}_\theta^{-1} = T_{\text{Rot}_\theta v}$$

is also in the translation subgroup. Thus, $v - \text{Rot}_\theta v$ is also in the translation lattice. Since v was the shortest nonzero vector in the translation lattice, we have

$$\|v - \text{Rot}_\theta v\| \geq \|v\|,$$

i.e. $\sin(\theta/2) \geq 1/2$. If $\theta = 1/n$ for a positive integer n , then this implies $n \geq 6$.

- **Example:** The 5 geometrically distinct 2-D lattices (parallelogram, square, rectangular, rhombic, hexagonal) and their point groups (Gallian Figure 28.20). Whether or not these full symmetry groups are retained depends on what is placed in the fundamental region of the lattice.

• The Plane Crystallographic Groups:

- There are 17 different plane crystallographic groups. This holds whether our notion of equivalence between $\text{Isom}(F_1)$ and $\text{Isom}(F_2)$ is group isomorphism, or “geometric equivalence” (the groups are identical under an affine-linear change of coordinates).

- Gallian Figure 28.18 gives a flowchart for classifying plane figures of these 17 groups.
Let's apply this to our Si(100) examples.

4 Using Symmetry to Understand Physical Properties

- Any physical property of a molecule or crystal must be invariant on its symmetry group.
- For example, let $\gamma : \mathbb{R}^2 \rightarrow \mathbb{R}$ be a scalar quantity giving some physical property of F at each point such as the surface energy or line energy density. Then it must hold that $\gamma \circ T = \gamma$ for every T in the symmetry group of F . Note that it suffices to impose this condition just for a set $\{T_1, \dots, T_k\}$ of *generators* of the symmetry group G , i.e. $G = \langle T_1, \dots, T_k \rangle$. This reduces the number of degrees of freedom in h .
- For example, the symmetry group of the square lattice has generators $\text{Rot}_{\pi/2}$, Ref_0 , $T_{(1,0)}$ and $T_{(0,1)}$. This imposes the following constraints on γ :

$$\begin{aligned}\gamma(x, y) &= \gamma(y, -x) \\ \gamma(x, y) &= \gamma(-x, y) \\ \gamma(x, y) &= \gamma(x + 1, y) \\ \gamma(x, y) &= \gamma(x, y + 1)\end{aligned}$$

Group theory (specifically, the theory of group representations) characterizes the form of possible functions h that can satisfy the above conditions.

- Many physical quantities of interest, such as electric fields and current density, are not scalars but *vector fields* $h : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ (or $h : \mathbb{R}^3 \rightarrow \mathbb{R}^3$). Two examples of interest in surface physics are the *mass flux* $J : \mathbb{R}^2 \rightarrow \mathbb{R}^2$, which gives the amount and direction of flow of a substance at a point on the surface, and the *concentration gradient* $\nabla\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^2$. The relation between these two quantities is a physical property of the crystal known as the *diffusivity* D , which is a 2×2 matrix. *Fick's Law* says that $J = -D\nabla\phi$. That is, for every $(u, v) \in \mathbb{R}^2$, we have:

$$\begin{pmatrix} J_x(u, v) \\ J_y(u, v) \end{pmatrix} = - \begin{pmatrix} D_{xx} & D_{yx} \\ D_{xy} & D_{yy} \end{pmatrix} \begin{pmatrix} (\nabla\phi)_x(u, v) \\ (\nabla\phi)_y(u, v) \end{pmatrix}.$$

- Note that we are assuming that the diffusivity D has no dependence on the position u, v (which is reasonable because diffusion is a macroscopic property). Thus its behavior is automatically invariant under translation. However the point group still imposes additional constraints on D . Specifically, if we apply a symmetry element $A \in \text{Point}(F, (0,0))$ to the concentration gradient $(\nabla\phi)(0,0)$ at zero, then we should get current density $AJ(0,0)$. So

$$-DA(\nabla\phi)(0,0) = AJ(0,0) = A(-D(\nabla\phi))(0,0).$$

Since this holds for all vectors $\nabla\phi(0,0)$, we have

$$DA = AD$$

(or equivalently $ADA^{-1} = D$).

For example, if the point group at 0 were D_4 (as in the square lattice, or the unreconstructed Si(100) face if we treat atoms at different heights as equivalent), then taking $A = \text{Rot}_{\pi/2} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, we get the following constraints on σ :

$$\begin{pmatrix} -D_{yx} & D_{xx} \\ -D_{yy} & D_{xy} \end{pmatrix} = \begin{pmatrix} D_{xy} & D_{yy} \\ -D_{xx} & -D_{yx} \end{pmatrix},$$

which tells us that $D_{xx} = D_{yy}$ and $D_{xy} = -D_{yx}$.

Taking $A = \text{Ref}_0$, we get:

$$\begin{pmatrix} -D_{xx} & D_{yx} \\ -D_{xy} & D_{yy} \end{pmatrix} = \begin{pmatrix} -D_{xx} & -D_{yx} \\ D_{xy} & D_{yy} \end{pmatrix},$$

which tells us that $D_{xy} = D_{yx} = 0$. Thus we conclude that D is simply of the form:

$$D = \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix},$$

i.e. the diffusivity is a fixed constant, independent of direction. When a physical property is independent of direction like this, it is called *isotropic*. On the other hand, in the case of the Si(100) surfaces (either the reconstructed case, or the unreconstructed case if we treat atoms at different heights as inequivalent), the point group is generated by Ref_0 and $-I$. The latter commutes with every matrix, and hence imposes no additional constraints. Thus, we can only conclude that the diffusivity is a diagonal matrix, but it may have different constants of proportionality in the x and y directions. That is, in this case, the diffusivity may be *anisotropic*.