AM 106: Applied Algebra	Salil Vadhan
Lecture Notes 15	
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- Reading: Gallian Chs. 27, 28.

1 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 $T : \mathbb{R}^n \to \mathbb{R}^n$ 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 $F : \mathbb{R}^n \to X$, the *symmetry group* of F is the set $\text{Isom}(F)$ of isometries $T : \mathbb{R}^n \to \mathbb{R}^n$ 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 $\text{Isom}(F)$.

- Let's calculate these subgroups for our Si(100) examples.

2 Crystallographic Groups

- **Def:** A *2-D crystal* is an infinite arrangement $F : \mathbb{R}^2 \to X$ of molecules or atoms such that $\text{Trans}(F)$ 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 $F : \mathbb{R}^2 \to X$ is a 2-D crystal and $p \in \mathbb{R}^2$, then every rotation in $\text{Point}(F, p)$ is of order 1, 2, 3, 4, or 6. Hence $\text{Point}(F, p)$ is isomorphic to $\mathbb{Z}_n$ or D_n for $n \in \{1, 2, 3, 4, 6\}$.

  Proof sketch: 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. (It is a fact that every lattice has a shortest nonzero vector, but we do not prove it here.) 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. $\sin(\theta/2) \geq 1/2$. Thus, $\text{Point}(F, 0)$ contains no rotations of angle smaller than $2\pi/6$. This implies that all rotations in $\text{Point}(F, 0)$ have angles of the form $2\pi k/n$ for $n \leq 6$ and $k \in \{0, 1, \ldots, n-1\}$. (A rotation of any other angle will generate a rotation of angle strictly between 0 and $2\pi/6$.) If $\text{Point}(F, 0)$ has only reflections then it will be isomorphic to $\mathbb{Z}_n$, and if it has a reflection then it will be isomorphic to D_n. (Composing two reflections with angles θ_1 and θ_2 gives a rotation with angle $\theta_1 - \theta_2$, so all of the reflections in the point group will have angles that differ by a multiple of $2\pi/n$.)

- **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 cystallographic 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.

3 Using Symmetry to Understand Physical Properties

- Any physical property of a molecule or crystal must be invariant on its symmetry group.

- For example, let $\gamma : \mathbb{R}^2 \to \mathbb{R}$ be a scalar quantity giving some physical property of F at each point such as the surface energy or line energy density. Then it most 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 $\{T_1, \ldots, T_k\}$ of *generators* of the symmetry group G, i.e. $G = \langle T_1, \ldots, T_k \rangle$. 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.

- One important physical property of a crystal is the the *diffusivity D*, which is a 2×2 matrix that relates two vector fields related to a substance on the surface of the crystal. One of these vector fields is the *mass flux J*, which the amount and direction of flow of a substance at a point on the surface, and the other is the *concentration gradient $\nabla \phi : \mathbb{R}^2 \to \mathbb{R}^2$*, which describes the direction in which the concentration of the substance is increasing. *Fick's Law* says that $J = -D\nabla\phi$.

- 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 change coordinates using any symmetry element $A \in \text{Point}(F, (0,0))$, the diffusivity should not change. That is, $ADA^{-1} = D$, or equivalently, $AD = DA$.

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 D:

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

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*.