Mathematical Foundations of Crystallography

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What are Crystals?

- “Regular Arrangements” of Atoms/Molecules in Solids.
- Question: What kinds of arrangements are possible?
- Answer: Use Group Theory to describe the possibilities.
Applied Group Theory

- “Groups” model concepts of symmetry.
- Set of objects w/ a binary operation such that:
  - An identity element e exists: \( ge = eg = g \)
  - There exist inverses: \( g(g^{-1}) = (g^{-1})g = e \)
  - Operation is associative: \( (gh)k = g(hk) \)
Group Examples

- $\mathbb{Z} = \{\ldots, -3, -2, -1, 0, 1, 2, 3, \ldots\}$
- Orthogonal Group $O(n)$
- Matrix Groups:
  - $GL(n, \mathbb{C}) = \{A \text{ a complex invertible matrix}\}$
  - $SL(n, \mathbb{C}) = \{A \in GL(n, \mathbb{C}) \mid \det(A) = 1\}$
Orthogonal Group

Definition:

- A 2x2 real matrix $A$ is orthogonal if:
  $$AA^T = A^TA = I \quad (i.e. \ if \ A^T = A^{-1}).$$
- Let $\|x\|$ be the length of vector $x$. A distance preserving linear transformation $T$ is said to be **orthogonal**. Such transformations form the **orthogonal group** $O(n)$. 
Subgroups of the Orthogonal Group

- An example of a subgroup of the orthogonal group is rotation about the origin on the plane:
Subgroups

- Non-empty subsets $H$ are subgroups if:
  - $h,k \in H \rightarrow hk \in H$ (closure)
  - $h \in H \rightarrow (h^{-1}) \in H$ (inverses)

- Examples:
  - $\mathbb{Z}_3 = \{0,1,2\}$ is a subgroup of the integers
  - $SL(n,\mathbb{R}) = \{A \in GL(n,\mathbb{R}) \mid \det(A) = 1\}$ is a subgroup of the General Linear group $GL(n,\mathbb{R})$. 
Equivalence Classes

“~” is an equivalence relation if it is:

- Reflexive: \( h \in G, \ h \sim h \)
- Symmetric: \( h, k \in G, \ h \sim k \rightarrow k \sim h \)
- Transitive: \( h \sim k, k \sim g \rightarrow h \sim g \)
An equivalence class is defined as a subset of the form \( \{ x \in G \mid x \sim y \} \), where \( y \) is an element of \( G \) and the notation "\( x \sim y \)" is used to mean that there is an equivalence relation between \( x \) and \( y \).

Equivalence classes are maximal sets of equivalent elements.
Example of Equivalence Class

- $\mathbb{Z}_3$ (Z “mod” 3)
- In this world, two elements are equivalent if their difference is divisible by three.
Coset Partitioning

- The concept of partitioning a group $G$ allows a better understanding of the structure of $G$ by breaking the group into parts (e.g. left cosets).

- A subset of $G$ of the form $gH$ for some $g \in G$ is said to be a left coset of $H$.
  - $gH = \{ gh \mid h \in H \}$
Example of Coset Partitioning

- Example: $G$ can be partitioned by cosets, also by conjugacy classes.
Conjugacy Classes

- Given G (any group), we say that for $h, k, g \in G$, $h \sim k$ ("$h$ is conjugate to $k$") if $k = ghg^{-1}$. This is known as conjugation.
- A conjugacy class is an equivalence class.
- In this case, equivalence classes are called conjugacy classes.
Conjugacy Classes cont’d.

- Each element in a group belongs to exactly one class, and the identity element ‘e’ is always its own conjugacy class.
The Full Symmetric Group $S_X$

- Let $X$ be a set.
- $S_X$ is the set of all 1:1 and onto maps of the set $X$ onto itself.
- The permutation groups are subgroups under $S_X$. 
Permutation Groups

- Definition: A permutation group is a subgroup of the group $S_X$.
- Permutation groups are otherwise known as transformation groups.
Examples of Permutation Groups

- The Symmetric Group for the natural numbers ($S_N$).
- The Dihedral Group ($D_n$).
- The Alternating Group ($A_n$).
Symmetric Group $S_N$

- $S_N$ is the full symmetric group for the natural numbers.
- Example: $S_3$ is the set of all self-bijections of $X = \{1,2,3\}$. 
Permutation

- A permutation is a rearrangement of an ordered list, let’s say S, into a 1:1 correspondence with S itself.
- The number of different permutations in a set of order n is n factorial (written n!).
An Example of Permutation Notation

\[
\begin{pmatrix}
1 & 2 & 3 \\
1 & 3 & 2
\end{pmatrix}
\]
Permutation Example

- Let’s look at the set $S = \{A, B, C\}$.
- The order of its permutation is:
  \[ n! = 3 \times 2 \times 1 = 6. \]
Permutation Example cont’d.

- The elements of S’s permutation are:
  - ABC
  - ACB
  - BAC
  - BCA
  - CAB
  - CBA
Cycle Notation

- First introduced by the great French mathematician Cauchy in 1815.
- Has theoretical advantages in that certain important properties of the permutation can be readily determined when cycle notation is used.
Permutation

- The act of changing the linear order of objects in a group.
Examples of Elements of $S_6$
Permutation Notation

\[
\left( \begin{array}{cccccc}
1 & 2 & 3 & 4 & 5 & 6 \\
2 & 3 & 4 & 5 & 6 & 1 \\
\end{array} \right)
\]
1-Cycle Notation

(1 2 3 4 5 6)
Permutation Notation

\[
\begin{pmatrix}
1 & 2 & 3 & 4 & 5 & 6 \\
4 & 3 & 2 & 5 & 6 & 1
\end{pmatrix}
\]
2-Cycle Notation

(1 4 5 6) (2 3)
Concepts of Cycle Notation

- Don’t need to write cycles that have only one entry. The missing element is mapped to itself.
- In a sense, the “order” does not matter.
G-Equivalence

- Permutation groups induce G-Equivalence.
- Suppose we have a permutation group G, where $G \subseteq S_X$.
- If $x, y \in X$, we say that $x$ and $y$ are “G-Equivalent” ($x \sim y$) if $gx = y$ for some $g \in G$. 
G-Equivalence cont’d.

- Fact: “G-Equivalence” is an equivalence relation.
- Definition: The equivalence classes of $X$ under the equivalence relation “$\sim$” are called $G$-orbits (or orbits).
Orbits

- Definition of orbit:
  \[ Gx = \{ y \in X \mid y = gx \text{ for some } g \in G \} \].

- This is also called G-equivalence.

- All elements in X are G-equivalent if there is only one orbit. In this case, we say that the action of G is transitive.
Examples of Orbits

- Example of an element of the full symmetric group on the plane:
  \[ \gamma = \mathbb{R}^2 \rightarrow \mathbb{R}^2 \ (1:1, \text{ onto}) \].

- Rotation group about the origin.
Rotation Group About the Origin

The orbits are the concentric circles.

\[
\begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}
\]
Invariance and Symmetry Groups
Groups as Models of Geometric Symmetry

- Crystals are formed through repetition or clustering of crystal atoms.
- Symmetry groups of invariant permutations are the foundation of crystallography because it models symmetry of objects (specifically crystal atoms and molecules) using group theory.
What is Invariance of Objects Under Permutation?

Definition:
- Recall that $S_X$ is the set of all permutations on $X$.
- Suppose we have a set $Y \subseteq X$ and a group $G \subseteq S_X$. Then the subset $Y$ is “$G$-invariant” if $gY \subseteq Y$, where $gY = g(Y)$, the image of $Y$ under $G$, $\forall g \in G$. 
Invariance of objects under permutation

■ What does that mean?
  ◆ For any object on a plane, symmetric permutations (rotation, translation, and reflection) leave an object invariant if it preserves the motif of that object.
Invariance of objects under permutation

- Here $y$ is acted upon by $g(y)$ under reflection. As we can see although the position of $y$ has changed, its pattern remains unchanged.
Specifically what are symmetry groups of objects?

- Symmetry groups are the consequence of an invariant permutation on a plane.
- e.g. Triangle permutations (D₃)
  - R₀, R₁₂₀, R₂₄₀
  - Reflection: R₁, R₂, R₃
  - Example of a permutation that is not invariant on D₃ is R₉₀
Symmetry Group of a Square

Or, the dihedral group of a square
Motivation

- Knowing conjugacy classes and valid geometric transforms allows easier modeling for computer applications by reducing the number of transformations that the computer needs to deal with.
Why is the Dihedral Group a Group?

- The dihedral group is a subset of the full symmetric group.
- Show each element has an inverse.
- Show that the group is closed under the operation.
Elements of the dihedral group

- Group elements: \{e, r, r^2, r^3, v, h, m, n\}
- \(e\) = identity (no transformation)
- \(r\) = 90° CCW rotation
- \(r^2\) = 180° CCW rotation
- \(r^3\) = 270° CCW rotation
- \(h\) = horizontal reflection
- \(v\) = vertical reflection
- \(m\) = reflection across main diagonal
- \(n\) = reflection across minor diagonal
Cayley Table for the Dihedral Group

<table>
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<tr>
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Inverses of the Elements of the Dihedral Group

- \( r^{-1} = r^3 \)
- \( r^{-2} = r^2 \)
- \( r^{-3} = r^1 \)
- \( h^{-1} = h \)
- \( v^{-1} = v \)
- \( m^{-1} = m \)
- \( n^{-1} = n \)
- \( e^{-1} = e \)
Conjugacy Classes

- Recall that an equivalence class is a subset of a group whose members are equivalent under some operation.
- A conjugacy class is a set whose members are equivalent under conjugation ($ghg^{-1}$) for $g, h \in G$.
- Thus, a conjugacy class is a way to partition a group into equivalence classes.
Determining Conjugacy Classes

- **Technique 1:** Pick \( h, k \in G \). \( h \sim k \) if \( k = ghg^{-1} \) for some \( g \in G \).

- **Technique 2:** Consider the conjugacy class as an orbit. Pick \( h \in G \), then find the conjugation \( \forall g \in G \). This will give the conjugacy class for \( h \).
Dihedral Group Conjugacy Classes

- Conjugacy classes of the dihedral group:
  \{ \{ e \}, \{ r, r^3 \}, \{ r^2 \}, \{ h, v \}, \{ m, n \} \}

- To find these, we will use Technique 2: select an \( h \in G \), then find the conjugation.
Finding the Conjugacy Classes

- Pick $r$. I claim that $\{ r \sim r^3 \}$.
- $r^3 rr^{-3} = r$
- $r^2 rr^{-2} = r$
- $h r h^{-1} = r^3$
- $v r v^{-1} = r^3$
- $m r m^{-1} = r^3$
- $n r n^{-1} = r^3$
- Thus $\{ r, r^3 \}$ is one conjugacy class.
- A similar procedure gives us the remainder of the conjugacy classes.
Impact on Crystallography

- Crystallographers study the geometric structure of crystals in many materials in order to determine a material’s physical properties, which benefits society as a whole.

- Knowing these conjugacy classes (i.e. knowing that certain transformations are equivalent) can speed up their computer analyses of the material.
References


■ “General Chemistry” by Linus Pauling, Dover 1970

Questions?