Lecture 1 | Welcome to Phys 5986TC

"Topology and Geometry in Modern Electronic Structure Theory"

Goals: 1. Understanding of the foundations of group theory in solid state physics

2. Develop tools to analyze research papers on topological materials

3. Learn to apply Berry phase techniques

to analyze electronic properties of solids

Rough guide to topics

1. Space group symmetries
2. Berry phases and Wannier functions
3. Band topology
4. Topological Crystalline insulators

course website: courses.physics.illinois.edu/phys598gtc

course components: - HW (5)

- class participation
- final presentations

Office hours: - TBD - zoom

- TA - Yuntao Guan 2pm-3pm Thursdays 3rd floor ESB

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① Review/Introduction to Group Theory

Useful Resources

- Dresselhaus "Applications of group theory to the physics of solids

- Serre "Linear representations of finite groups"
- Bradley and Cracknell "Mathematical Theory of symmetry in solids"

Starting point: $H = \frac{\vec{p}^2}{2m} + V(\vec{x}) + \dots$

Schrödinger equation $H|\psi\rangle = E|\psi\rangle$

transformations $\vec{x} \to \vec{x}'$ $\quad |\psi\rangle \to |\psi'\rangle$

$\vec{p} \to \vec{p}'$

Symmetries: transformations $H \to H' = H$

This course: mainly interested in transformations of space

$$\vec{x} \to \vec{x}' = R\vec{x} + \vec{d}$$

$$\vec{p} \to \vec{p}' = R\vec{p}$$

R - 3x3 matrix rotation or reflection

$R^T = R^{-1}$ ← orthogonal

$\vec{d}$ - translation vector

Basic Facts:

① $\vec{x} \to \vec{x}' = \vec{x}$
$\vec{p} \to \vec{p}' = \vec{p}$ ← transformation where I do nothing - "Identity transformation"

2. I can always undo a transformation ← consider transformations that have inverses

3. If I have two transformations, I can compose them to get a third

→ Define: a set G is a <u>group</u> if

1. there's an operation $\cdot$ (product) such that

$$g_1 \in G,\ g_2 \in G \quad g_1 \cdot g_2 \in G$$

$$g_1 \cdot (g_2 \cdot g_3) = (g_1 \cdot g_2) \cdot g_3 \quad \text{(associative)}$$

2. there exists $E \in G$ such that

$E \cdot g = g \cdot E = g$ for all $g \in G$

3. if $g \in G \Rightarrow$ there exists g^{-1} s.t.

$g \cdot g^{-1} = g^{-1} \cdot g = E$

Examples of groups:

1. Unitary operators on (d-dimensional) Hilbert space

$U(d)$ - the set of $d \times d$ matrices $V \in U(d)$

$V^{\dagger} = V^{-1}$

- Binary operation - matrix multiplication
- Identity matrix $\mathbb{1}$ is E
- unitary matrices all have inverses

$V_1, V_2 \in U(d)$

$$(V_1 V_2)^\dagger = V_2^\dagger V_1^\dagger = (V_1 V_2)^{-1}$$

(2) The group of rotations in 3d space

special orthogonal group $SO(3)$

special: determinant 1

orthogonal: transpose is inverse

(3): 3x3 matrices

(3) Translations in 3D space $\mathbb{R}^3$

- elements are 3d vectors $\vec{v} \in \mathbb{R}^3$
- binary operation: vector addition
- identity is $\vec{0}$
- inverses: $v^{-1} = -v$

$$\vec{x} \to \vec{x}' = \vec{x} + \vec{v}$$

Some important facts about groups

- Given a group G we can consider subsets

$H \subseteq G$ such that H is also a group

(subgroups $H \leq G$ ("H is a subgroup of G")

$H \subseteq G$ is a subgroup if:

- $E \in H$
- H is closed under $\cdot$: $h_1, h_2 \in H \Rightarrow h_1 h_2 \in H$
- H is closed under taking inverses $h \in H$
  $\Rightarrow h^{-1} \in H$

Examples: • Group $SO(3)$ and pick some axis $\hat{n}$

$\{$all rotations about $\hat{n}\} \subset SO(3)$

$$\begin{array}{c} \parallel \\ SO(2) < SO(3)) \end{array}$$

- translation group $\mathbb{R}^3 = \{(x,y,z) \mid x,y,z \in \mathbb{R}\}$

  pick 3 linearly independent vectors $\vec{t}_1, \vec{t}_2, \vec{t}_3$

$$T = \{n_1\vec{t}_1 + n_2\vec{t}_2 + n_3\vec{t}_3 \mid n_1, n_2, n_3 \in \mathbb{Z}\}$$

$T < \mathbb{R}^3 \leftarrow$ subgroups of this form are called Bravais lattices

$H \leq G$ - H is a subgroup of G (H could be G itself)

$H < G$ - H is a "proper subgroup" (H is a subgroup of G
$H \neq G$)

We can use subgroups $H \leq G$ to learn about the structure of G:

given G a group $H \leq G$ a subgroup
we can define, for each $g \in G$, the right coset of H by g

$$Hg = \{h \cdot g \mid h \in H\}$$

Important fact: Every element $g' \in G$ is in one and only one right coset of H

Proof: First show that every $g' \in G$ is in at least one right coset, then show its in only one

1. Remember $E \in H$

$$Hg' = \{h \cdot g' \mid h \in H\} \ni E \cdot g' = g'$$

2. Now we show this is the only one:

assume $g' \in Hg_1$ and $g' \in Hg_2$ $g_1 \neq g_2$

and show $Hg_1 = Hg_2$

$g' \in Hg_1$ $\quad$ $g' \in Hg_2$

$\downarrow$ $\quad$ $\downarrow$

$g' = h_1 \cdot g_1$ $\quad$ $g' = h_2 \cdot g_2$

$h_1 g_1 = h_2 g_2$

$h_1^{-1} h_1 g_1 = h_1^{-1} h_2 g_2$

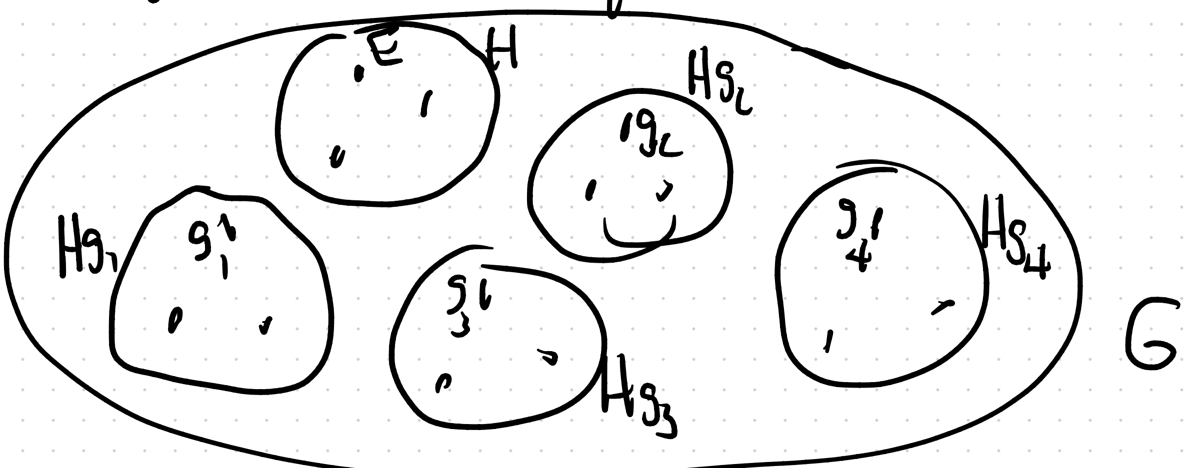
$g_1 = (h_1^{-1} h_2) \cdot g_2$ $\quad$ $h_1^{-1} \cdot h_2 \in H$

$Hg_1 = \{hg_1 \mid h \in H\}$

$= \{ h \cdot (h_1^{-1} h_2)\, g_2 \mid h \in H \}$ $\quad h' = h \cdot h_1^{-1} h_2$

$= \{ h' \cdot g_2 \mid h' \in H \} = Hg_2$ $\quad$ group multiplication is invertible

→ every element of G is in exactly one right coset –
right cosets of H partition G



$G = H(E) \cup Hg_1 \cup Hg_2 \cdots \cup Hg_{n-1}$ ← coset decomposition of G

$\{ \underset{g_0}{\overset{\shortparallel}{E}}, g_1, g_2 \cdots g_{n-1} \}$ ← coset representatives

n - total # of right cosets of H - the <u>index</u> of H in G $n = |G : H|$

The <u>number</u> of coset representatives is fixed, but the representatives themselves are not unique

$Hg_i = H(hg_i)$

g_i and hg_i have to be in the same coset

let $h' \in H$

$Hh' = \{hh' \mid h \in H\}$

$= H$