Lecture 1

Welcome to Phys 598 GTC

"Modern Electronic Structure Theory"

Goals:

1. Understand the foundations of group theory in solid state physics
2. Develop tools to analyze & evaluate research papers on topological materials
3. Learn to apply Berry phase techniques to analyze electronic properties of topological materials

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) ← graded on completeness
- Class participation

- Final presentations

Office hours: TBD via Zoom

I. Review of / Intro to Group Theory

Useful Resources

- Dresselhaus "Applications of group theory to the physics of solids."
- Bradley & Cracknell "Mathematical Theory of Symmetry in solids"

· Serre "Linear representations of finite groups"

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

Schrödinger Eqn: $H|\psi\rangle = E|\psi\rangle$

Find transformations:

$$\vec{x} \to \vec{x}'$$
$$\vec{p} \to \vec{p}'$$
$$|\psi\rangle \to |\psi'\rangle$$

Symmetries: transformations that leave the Schrödinger Eqn unchanged $H \to H' = H$

This course is mainly interested in transformations of space

$$\vec{x}\,' = R\vec{x} + \vec{d} \qquad R - 3\times3 \text{ rotation or reflection}$$

$$\vec{p}\,' = R\vec{p} \qquad R^{-1} = R^T \leftarrow \text{orthogonal}$$

$\vec{d}$ ~ translation vector

Basic Intuitive Facts:

1. If I have two transformations, I can first do one transformation and then

do the other. This is also a transformation

(2) $\vec{x} \to \vec{x}$, $\vec{p} \to \vec{p}$ is a transformation - identity transformation

(3) We can always undo a transformation - inverse transformations exist

<u>Definition</u> a set G is called a <u>group</u> if:

(1) there is a binary operation $\cdot$ (product) s.t. for any $g_1 \in G$, $g_2 \in G$,

$g_1 \cdot g_2 \in G$ and $g_1 \cdot (g_2 \cdot g_3) = (g_1 \cdot g_2) \cdot g_3$

② there exists $E \in G$ s.t. for all $g \in G$

$E \cdot g = g \cdot E = g$ $\quad$ E is the identity element

③ if $g \in G$, 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 $V \in U(d)$ s.t.

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

- Binary operation: matrix multiplication

$V_1^\dagger = V_1^{-1} \quad V_2^\dagger = V_2^{-1}$

$(V_1V_2)^\dagger = V_2^\dagger V_1^\dagger = V_2^{-1}V_1^{-1} = (V_1V_2)^{-1}$

- E is $d \times d$ identity matrix
- inverses by construction

② The group of rotations in 3D

the special orthogonal group $SO(3)$

special: det 1

orthogonal: transpose is inverse

(3): 3×3 matrices

③ Translations in 3D $\mathbb{R}^3$

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

each $v \in \mathbb{R}^3$ defines a transformation $\vec{x} \to \vec{x} + \vec{v}$

"H is a subset of G"

Some important facts about groups:

Given a group G we can consider subsets $H \subseteq G$

such that H is also a group $\leftarrow$ <u>subgroup</u> $H \leq G$

H is a subgroup if: $\cdot\ E \in H$ "H is a subgroup of G"

$\cdot$ H is closed under multiplication

$h_1 \in H,\ h_2 \in H,\ h_1 \cdot h_2 \in H$

$\cdot$ H is closed under inverses

$h \in H \Leftrightarrow h^{-1} \in H$

Examples: consider $SO(3)$ and consider: fix $\hat{n}$

$$\underbrace{\{\text{rotations about the axis } \hat{n}\}}_{\cong\ SO(2)\ <\ SO(3)} \subset SO(3)$$

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

G is a subgroup of G. If H is a subgroup of G AND $H \neq G$ then we say H is a <u>proper subgroup</u> of G

$H \leq G$ - H is a subgroup of G

$H < G$ - H is a proper subgroup of G

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

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

$T < \mathbb{R}^3$ ← subgroups of this form are called <u>Bravais lattices</u>

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

Given a group G and a subgroup H, we can define, for any $g \in G$ a <u>right coset</u> of H

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

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

Proof: First, we want to show that every $g' \in G$ is in at least one right coset. Recall $E \in H$

$$Hg' = \{hg' \mid h \in H\} \ni Eg' = g'$$

to show this is the only one we need to show that

$g' \in Hg_1$ and $g' \in Hg_2 \Rightarrow Hg_1 = Hg_2$

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

$h_1 g_1 = h_2 g_2$

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

$\Rightarrow h_2^{-1} h_1 = g_2 g_1^{-1} \in H$

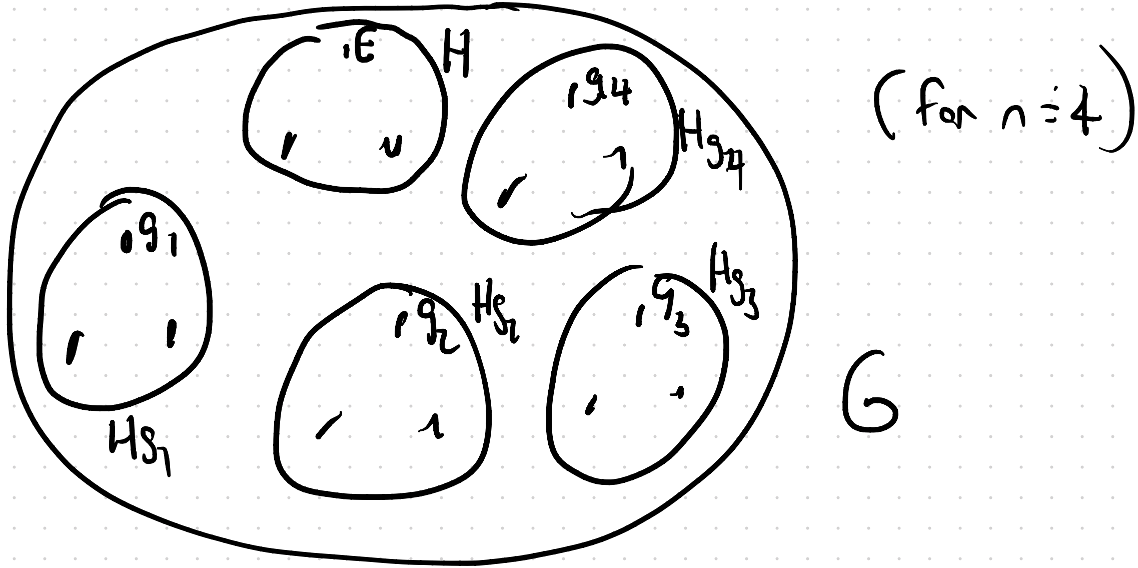
H is closed under multiplication: $Hg_2g_1^{-1} = H$

$$Hg_2 = Hg_1$$

$\Rightarrow$ every element of G is in exactly one right coset – right cosets of H partition the group

$$G = H \cup Hg_1 \cup Hg_2 \cdots \cup Hg_{n-1}$$ ← n right cosets

"coset decomposition"



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

n - number of right cosets the index of H in G $n = |G : H|$

Sylow