Lecture 1 | # Welcome to Phys 598 GTC

Goals for the course:

- Develop theory background for research in topological materials
- Understand modern developments in the study of noninteracting electrons
- Develop a foundation for understanding group theory in solid state physics

Guide to topics:

1. Space group symmetries
2. Wannier functions and band representations
3. Berry phases and band topology
4. Topological crystalline insulators

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

Course Components: Lectures

HWs (5) ← graded on completeness
submitted via gradescope

Final presentations

Office hours: 4-5pm Mondays via Zoom link
on course website

I. Review/Intro to Group theory

Useful resources:

- Dresselhaus "Applications of Group Theory to the Physics of Solids"

- Bradley & Cracknell "Mathetical Theory of Symmetry in solids"

- Serre "Linear Representations of Finite Groups"

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

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

Find the set of transformations
$\vec{x} \to \vec{x}'$

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

$$|\psi\rangle \to |\psi'\rangle$$

that leave the Schrödinger equation unchanged

$$H \to H' = H$$

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

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

R - 3x3 rotation or reflection matrix $R^T = R^{-1}$

$\vec{d}$ - translation vector

Intuitive Facts: ① if I have two transformations, I can do one and then the other to get a third transformation

(2) I can always undo a transformation

(3) $\vec{x} \to \vec{x}$
$\vec{p} \to \vec{p}$ is a transformation

- identity transformation

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

(1) theres some binary operation $\cdot$ such that if
$g_1 \in G$, $g_2 \in G$, then $g_1 \cdot g_2 \in G$, and
$g_1 \cdot (g_2 \cdot g_3) = (g_1 \cdot g_2) \cdot g_3$

③ $E \in G$ s.t. for all $g \in G$ $E \cdot g = g \cdot E = g$

E is the <u>identity</u>

② If $g \in G$, then there exists g^{-1} such that $g \cdot g^{-1} = g^{-1} \cdot g = E$

Examples of Groups: ① The set of unitary operators on Hilbert space (d-dimensional)

$U(d)$

- The binary operation is Matrix multiplication
- $E =$ $d \times d$ identity matrix
- $V \in U(d)$, $V^\dagger \in U(d)$

  $V^\dagger V = E$
- $V_1 \in U(d)$, $V_2 \in U(d)$

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

  $\Rightarrow V_1 V_2 \in U(d)$

② The group of rotations in 3-dimensions "special orthogonal group" $SO(3)$

3×3 matrices, determinant 1, transpose is their inverse

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

- elements are vectors
- binary operation is addition of vectors

  $\vec{v} \in \mathbb{R}^3$ defines the transformation $\vec{x} \to \vec{x} + \vec{v}$
- identity element: $\vec{0}$
- inverses: $\vec{v}^{-1} = -\vec{v}$

Some important facts about groups

- Given a group G, we can consider subsets $H \subset G$ that are also groups ← H is a subgroup of G

$H \subset G$ is a subgroup if:

1. $E \in H$
2. H is closed under multiplication
3. H is closed under taking inverses: $h \in H \Rightarrow h^{-1} \in H$

Examples: · Consider $SO(3)$. Consider $SO(2) \subset SO(3)$

consisting of all rotations about a fixed axis $\hat{n}$

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

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

$$T = \{n\vec{t}_1 + m\vec{t}_2 + l\vec{t}_3,\ n,m,l \in \mathbb{Z}\}$$

integers

$T \subset \mathbb{R}^3$ is a subgroup known as a Bravais lattice

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

given a group G and a subgroup H we can define

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

$g \in G$

Important fact: every element $g' \in G$ is in exactly one right coset of H

proof: first: $E \in H$

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

so g' is in at least one right coset Hg'

to show it is only in one right coset; need to show $g' \in Hg_1$ and $g' \in Hg_2 \Rightarrow Hg_1 = Hg_2$

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

$$h_1 g_1 = h_2 g_2$$

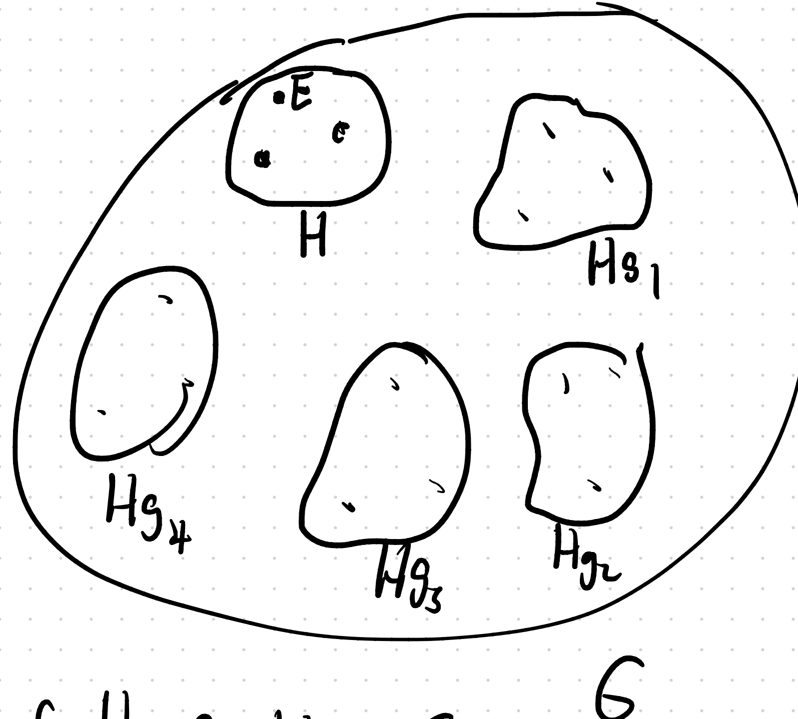
$$\Rightarrow h_2^{-1} h_1 g_1 = h_2^{-1} h_2 g_2$$

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

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

$$Hg_2 g_1^{-1} = H$$

$$\Rightarrow Hg_2 = Hg_1$$



Right cosets of H partition G

$$G = \overset{E}{H} \cup Hg_1 \cup Hg_2 \cdots \cup Hg_{n-1} \quad \leftarrow n \text{ right cosets of } H$$

n is known as the index of H in G $|G:H|$

$\{E, g_1, g_2, \dots g_{n-1}\}$ are coset representatives of H