Lecture 1 | Welcome to Phys 598 GTC

Goals for the course:

- Develop theoretical background for research on topological materials
- Understand modern developments in the theory 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 (~6)
Final Presentations

HWs graded primarily on completion rather than correctness

Office Hours: Mondays $\boxed{\text{will send a poll}}$ via Zoom link on course website.

I. Review/Refresher/Intro to Group Theory

Useful resources:
- Dresselhaus, "Applications of Group Thy to Physics of Solids"
- Bradley & Cracknell "Mathematical Thy of Symmetry in Solids"

- Serre "Linear Representations of Finite Groups"

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

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

$x \to x'$

$p \to p'$

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

In this course, we will be interested in transformations

$$\vec{x}' = R\vec{x} + \vec{d} \qquad R \text{ is a } 3\times 3 \text{ matrix}$$

$$\vec{p}' = R\vec{p} \qquad R^T = R^{-1}$$

Intuitive Facts: ① If I have two transformations, I can first do one then the other this is also a transformation

② I can always undo a transformation, and that's also a transformation

③ I can always do a transformation that does absolutely nothing

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

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

③ $E \in G$ such that $g \cdot E = E \cdot g = g$ for all $g \in G$. E is the <u>identity</u>

② If $g \in G$ then there exists $g^{-1} \in G$

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

Examples of groups: The set unitary operators on a d-dimensional Hilbert space is a group $U(d)$

- the binary operation is matrix multiplication
- $U_1^{\dagger} = U_1^{-1}$

- $U_1 U_2$ is unitary if U_1, U_2 unitary

- Rotations in 3D form a group (SO(3))
  special orthogonal group
  : determinant 1, 3×3 orthogonal rotation matrices

- Translations in 3D space form a group
  : binary operation is vector addition
  $\vec{V}_1, \vec{V}_2, \rightarrow \vec{V}_1 + \vec{V}_2$

- identity translation: $\vec{0}$
- inverseses $\vec{v}^{-1} = -\vec{v}$

Some important facts about groups:

- Given a group G, we can consider subsets $H \subset G$ that are also groups:

  $H \subset G$ is a <u>subgroup</u> if:

  1. $E \in H$
  2. H closed under multiplication

3. H closed under taking inverses

Examples:

- Consider the rotation group $SO(3)$. We can consider all rotations about some fixed axis $\hat{n}$. This is a subgroup $SO(2) \subset SO(3)$
- Consider $\mathbb{R}^3 = \{(x, y, z)\}$ 3D translation group. Pick 3 linearly independent vectors $\vec{t}_1, \vec{t}_2, \vec{t}_3$

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

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

We can learn about the structure of G from a subgroup H.

we can define a right coset $Hg = \{hg \mid h \in H\}$ for $g \in G$

Important fact: every $g' \in G$ 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 coset. Now we need to show that if $g' \in Hg_1$, $g' \in Hg_2$

$\Rightarrow Hg_1 = Hg_2$

$$g' \in Hg_1 \qquad g' \in Hg_2$$

$$\downarrow \qquad \downarrow$$

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

$$h_1 g_1 = h_2 g_2$$

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

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

$$H = Hg_2g_1^{-1} = \{hg_2g_1^{-1} \mid h \in H\}$$

$$Hg_1 = Hg_2$$

$$h' = hg_2g_1^{-1}$$

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

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

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

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

Example: 1D Bravais lattice $T = \{n\hat{x}, n \in \mathbb{Z}\}$