Lecture 1 | Welcome to Phys 567

Geometry & Topology in Modern Electronic Structure Theory

1. Understand the foundations of group thy in solid state physics

2. Develop tools to analyze research papers on topological materials

(3) Learn to apply Berry phase techniques to analyse electronic properties of solids

Rough guide to topics:

1. Space group symmetries
2. Berry phases & Wannier functions
3. Band topology / topological materials
4. Topology & "quantum geometry"

course website: courses.illinois.edu/phys567/fa2025

course components: 5 HWs
Final presentation

Office Hours: TBD

I. Review/Introduction to group theory

Useful references:
- Serre "Linear representations of Finite Groups"
- Dresselhaus "Application of Group Theory

to the Physics of Solids"

- Bradley & Cracknell "Mathematical Theory of Symmetry in Solids"

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

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

$x \to x'$ $|\psi\rangle \to |\psi'\rangle$
$p \to p'$

symmetries: transformations that take
$H \to H' = H$

This course: transformations of space

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

$$\rho \to \rho' = R\vec{x}$$

R - 3x3 matrix rotation or reflection

$\vec{d}$ - translation

Some intuitive facts

① I can always do nothing $x \to x$, $\rho \to \rho$ "identity transformation"

② I can always undo a transformation ⇐ transformations have inverses

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

Define a set G is a group if

① There is an operation $\cdot$ (product) such that
$g_1 \in G$ $g_2 \in G$ then $g_1 \cdot g_2 \in G$

$g_1 \cdot (g_2 \cdot g_3) = (g_1 \cdot g_2) \cdot g_3$ (associative)

② there exists $E \in G$ such that
$E \cdot g = g \cdot E = g$ for all $g \in G$

③ If $g \in G$ then there exists $g^{-1} \in G$

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

Examples of groups: ① Unitary operator on (d-dimensional) Hilbert space

- Binary operation: matrix multiplication
- E = $d \times d$ identity matrix
- Inverse - hermitian conjugate

$U(d)$

② The group of rotations of 3d space

$$SO(3)$$

special — $\det = 1$

orthogonal — transpose = inverse

3×3

③ Translations in 3D: $\mathbb{R}^3$

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

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

a special kind of subset is those where H is itself a group $\leftarrow$ "subgroups" $H \leq G$

$H \subseteq G$ is a subgroup if:

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

Example: $SO(3)$ rotation group pick an axis $\hat{n}$

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

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

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

$\parallel$

$SO(2) < SO(3)$

2d rotation group

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

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

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

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

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

Given $H \leq G$ we can define, for each $g \in G$, a <u>right coset</u> $Hg = \{h \cdot g \mid h \in H\}$

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

Proof: First: show that every $g' \in G$ is in at least one coset,
Second: show that it is in only one coset

1. Remember $E \in H \Rightarrow g \in Hg$

2. Need to show if $\underline{g' \in Hg_1}$ and $\underline{g' \in Hg_2} \Rightarrow$

$Hg_1 = \underline{Hg_2}$

$g' \in Hg_1$

$\downarrow$

$g' = h_1 \cdot g_1$

$g' \in Hg_2$

$\downarrow$

$g' = h_2 \cdot g_2$

$h_1, h_2 \in H$

$h_1 \cdot g_1 = h_2 \cdot g_2$

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

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

$$Hg_1 = \{h \cdot g_1 \mid h \in H\} \qquad Hg_2$$

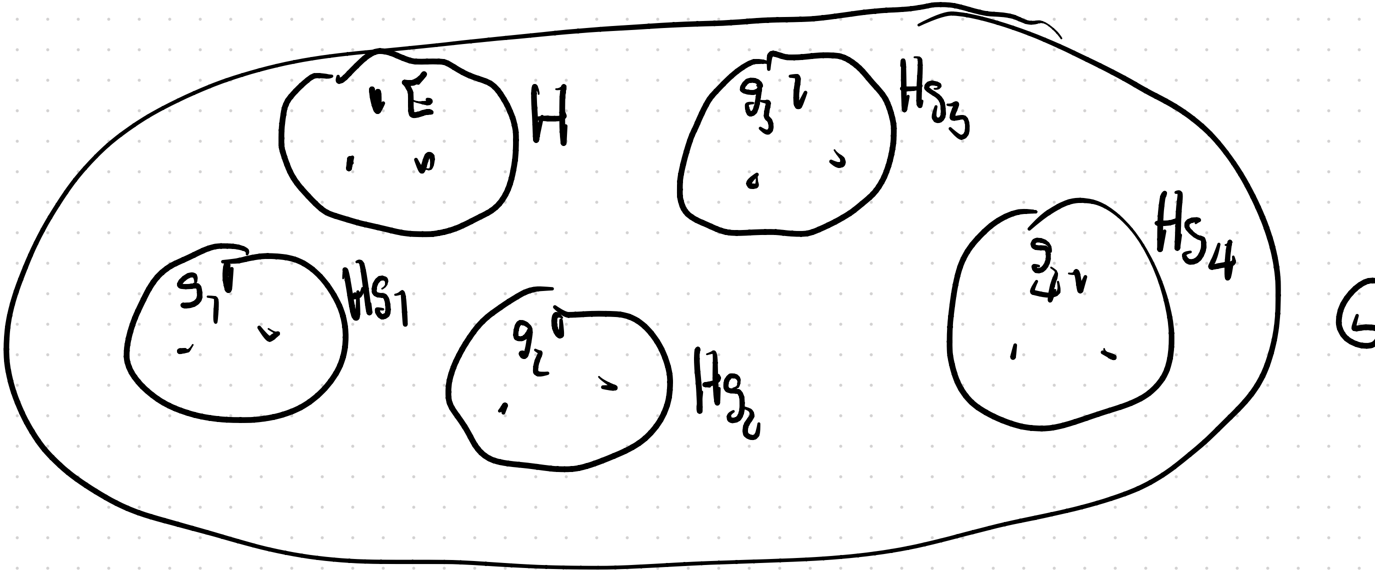
$$= \{h \cdot h_1^{-1} \cdot h_2 \cdot g_2 \mid h \in H\} = \{h' \cdot g_2 \mid h' \in H\}$$

remember: group multiplication is invertible

$$H \ni h' = h \cdot (h_1^{-1} \cdot h_2)$$

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

→ right cosets partition the elements of G



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

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

we will always choose this one $\{E, g_1, \dots, g_{n-1}\}$ - "coset representatives" to be Σ

coset representatives are not unique

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

$$= \{h\underbrace{(h' g_1)}_{g_1'} \mid h \in H\}$$