Lecture 1

Welcome to Phys 598 GTC

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

Goals:
- Background necessary to study topological materials
- Modern developments in the thy of non-interacting electronic solids
- Develop a foundation for starting to study strong correlations

Rough guide:

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

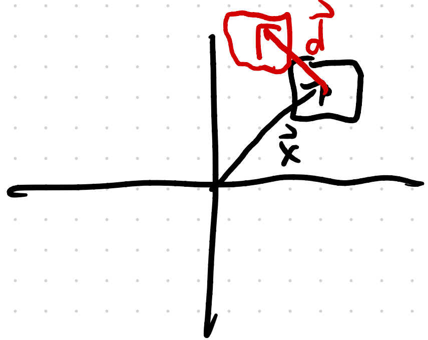
Office Hrs: 4pm-5pm Mondays

I. Point and Space groups

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

- Serre "Linear Representations of Finite Groups"

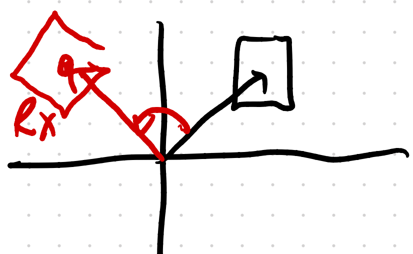
Transformations $\qquad$ d-dimensional space $(d = 1, 2, 3 \ldots)$



What are the rigid transformations that we can do to this object

translation $\vec{x} \to \vec{x} + \vec{d}$

we could also perform a rotation or reflection $\vec{x} \to R\vec{x}$



Any rigid transformation can be written as a combination $\{R|\vec{d}\}$ of a rotation/reflection with a translation

$\{R|\vec{d}\}$ - Seitz Symbol

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

$$\mathbb{E}(d) = \left\{ \{R|\vec{d}\},\ \vec{d} \in \mathbb{R}^d \text{ is a translation } R \in O(d) \right\}$$

Euclidean group

Orthogonal group

What does it mean for something to be a group?

$R \in O(d)$: $x_i \to R_{ij} \vec{x}_j$ $\qquad$ $R \in O(d) \Leftrightarrow |\det R| = 1$

(1) $R_1, R_2 \in O(d)$ $\qquad$ $\underline{R_1 R_2}$

$$|\det(R_1 R_2)| = |\det R_1 \det R_2| = |\det R_1||\det R_2| = 1$$

$$R_1 \in O(d),\ R_2 \in O(d) \Rightarrow R_1 R_2 \in O(d)$$

(2) $E = \left.\begin{pmatrix} 1 & & \\ & 1 & \\ & & \ddots \end{pmatrix}\right]d$ $\quad$ $d \times d$ identity matrix $\in O(d)$

$E\vec{x} = \vec{x}$

(3) R^{-1} exists and $|\det R^{-1}| = \dfrac{1}{|\det R|} = 1$

$R^{-1} \in O(d)$

$\Rightarrow$ $O(d)$ is a group

A <u>group</u> is any set G with a binary operation (multiplication) such that:

(1) There is an identity element $E \in G$

(2) The set is closed under the binary operation

③ every element has an inverse

$g \in G \quad g^{-1} \in G$ s.t. $gg^{-1} = E$

$O(d)$ is a group

Claim: the translations $\{\vec{d} \in \mathbb{R}^d\}$ is a group with binary operation $+$

①: $\vec{d}_1 \in \mathbb{R}^d$, $d_2 \in \mathbb{R}^d$ $\quad \vec{d}_1 + \vec{d}_2 \in \mathbb{R}^d$

②: $\vec{\emptyset} \in \mathbb{R}^d \quad \vec{d} + \vec{\emptyset} = \vec{d}$

③ $\vec{d} \in \mathbb{R}^d \Rightarrow -\vec{d} \in \mathbb{R}^d \quad \vec{d} + (-\vec{d}) = \vec{\emptyset}$

Let's show that $\mathbb{E}(d)$ is a group

$g_1 = \{R_1 | \vec{d}_1\} \quad g_2 = \{R_2 | \vec{d}_2\} \in \mathbb{E}(d)$

$$g_1 : \vec{x} \to R_1\vec{x} + \vec{d}_1 = g_1\vec{x}$$

$$\begin{aligned} g_2 g_1 : x \to g_2(g_1\vec{x}) &= g_2(R_1\vec{x} + \vec{d}_1) \\ &= R_2(R_1\vec{x} + \vec{d}_1) + \vec{d}_2 \\ &= R_2R_1\vec{x} + (R_2\vec{d}_1 + \vec{d}_2) \end{aligned}$$

$$= \{R_2R_1 \mid R_2\vec{d}_1 + \vec{d}_2\}\vec{x}$$

$$\{R_2 \mid \vec{d}_2\}\{R_1 \mid \vec{d}_1\} = \{R_2R_1 \mid R_2\vec{d}_1 + \vec{d}_2\} \in \mathbb{E}(d)$$

2. $\{E \mid \emptyset\}\vec{x} = \vec{x}$

$$\{E \mid \emptyset\}\{R \mid \vec{d}\} = \{ER \mid E\vec{d} + \emptyset\} = \{R \mid \vec{d}\}$$

$\Rightarrow \mathbb{E}(d)$ has an identity operation

3. We need to find the inverse of $\{R \mid \vec{d}\}$

$$\{R|\vec{d}\}^{-1} = \{A|\vec{t}\} \text{ for } A \in O(d),\ \vec{t} \in \mathbb{R}^d$$

$$\{E|\emptyset\} = \{A|\vec{t}\}\{R|\vec{d}\} = \{AR|A\vec{d}+\vec{t}\}$$

rotation parts $\quad E = AR \rightarrow A = R^{-1}$

translation parts $\quad \vec{\emptyset} = R^{-1}\vec{d} + \vec{t} \rightarrow \vec{t} = -R^{-1}\vec{d}$

$$\{R|\vec{d}\}^{-1} = \{R^{-1}|-R^{-1}\vec{d}\}$$

$\rightarrow$ $\mathbb{E}(d)$ is a group ✓✓✓

Every element $\{R|\vec{d}\} \in \mathbb{E}(d)$

$$\{R|\vec{d}\} = \underbrace{\{E|\vec{d}\}}_{\in\, \mathbb{R}^d} \underbrace{\{R|\emptyset\}}_{\in\, O(d)}$$

we say that $\mathbb{E}(d) = \mathbb{R}^d \rtimes O(d)$

semidirect product

$$\{R_1|\vec{d}_1\}\{R_2|\vec{d}_2\} = \{R_1R_2|R_1\vec{d}_2+\vec{d}_1\}$$

[on the contrary

$\mathbb{R}^d \times O(d)$

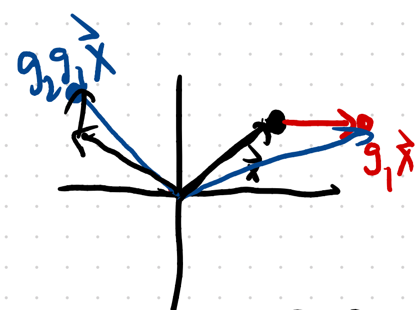
direct product

$(R_1,\vec{d}_1)(R_2,\vec{d}_2) = (R_1R_2, d_1+d_2)$]

Ex: 2D System

$g_1 = \{E|\hat{x}\}$

$g_2 = \{R_{\pi/2}|\emptyset\}$



$g_2g_1x = \{R_{\pi/2}|\hat{y}\}$

Lets start applying this to crystals

- Crystals are defined by the fact that they have discrete translation symmetry

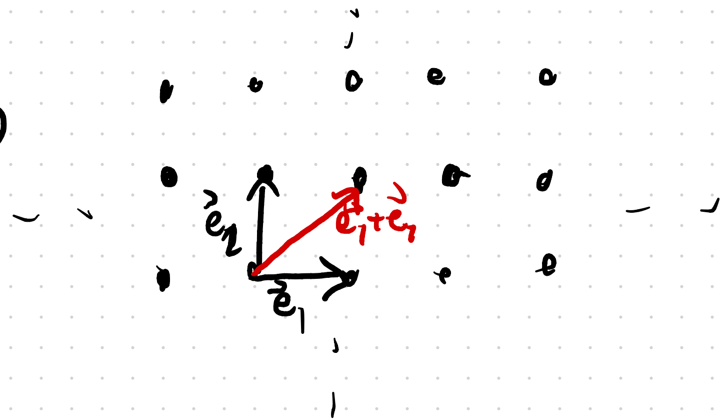
let G be the group of transformations that leave the crystal invariant

$G \subset \mathbb{E}(d)$ is a subgrp of the euclidean group

$$G \ni \{ E \mid n_1 \vec{e}_1 + n_2 \vec{e}_2 + \cdots n_d \vec{e}_d \}$$

$n_1, n_2, n_3 \cdots n_d \in \mathbb{Z}$ integers

Ex: 2D



$n_1 \vec{e}_1 + n_2 \vec{e}_2$ are symmetries of this lattice

Any discrete subgroup of $\mathbb{R}^d$ is generated by choosing a basis (for a d-dimensional xtal))

The set of translations

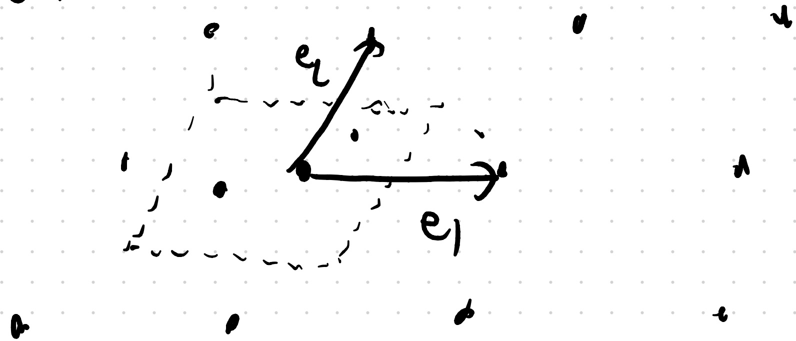
$$\{\{E \mid n_1\vec{e}_1 + n_2\vec{e}_2 + \cdots n_d\vec{e}_d\}\}$$ is called

the Bravais lattice of the crystal

any choice of $\{\vec{e}_1, \vec{e}_2, \ldots \vec{e}_d\}$ that generates the Bravais lattice is called a set of primitive lattice vectors

Given a choice of primitive lattice vectors, we can define a <u>primitive unit cell</u>:

a subset of space s.t. no lattice translation maps points inside the unit cell to other points in the unit cell



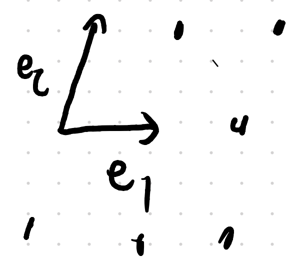
$\vec{x} \in PUC$ if $\vec{x} = t_1 \vec{e}_1 + t_2 \vec{e}_2 \quad t_1, t_2 \in \left(-\frac{1}{2}, \frac{1}{2}\right)$

Any choice of d linearly independent vectors defines a Bravais lattice

However for special choices of primitive lattice vectors, the Bravais lattice might have extra symmetry

Ex 2d

$$\vec{e}_1 = a\hat{x}$$
$$\vec{e}_2 = b\hat{x} + c\hat{y}$$



if $b = 0$

if $b = 0$ AND $a = c$