Day 1 Phys 58

- Introduce myself
- Introductions of class.
- Syllabus.
  - ~~textbook~~ (Ch 1-8, part of 9, part of 14)
  - hw
  - exam

Need substitute for 2 Mondays!

What is a solid? resist shear

- crystalline ★ This class!
- amorphous
- infinite ★
- finite (surfaces)

Crystal: periodicity (atoms)

1D: • • • •

what about •• •• •• •• ?

period — yes, is crystal

lattice — details of periodicity (abstract pts)

basis — details of atoms that are found at the lattice pts

Note lattice choice is not unique

lattice × × × ×
basis ••

=

lattice × × × ×
basis |—→••

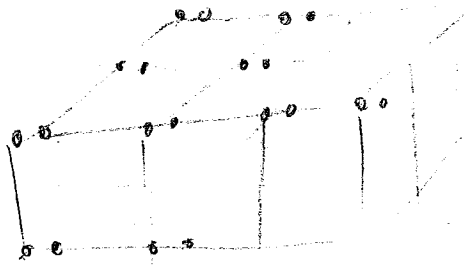
(but some choices are better than others)

best choice? × × × ×
•/•

↑ basis is symmetric, possibly best choice.

Symmetry! Mathematical techniques for analyzing symm = Grp. Theory (beyond this class)

3D



← could be crystal

lattice = "simple cubic"

basis? atom 1 at (0,0,0)
atom 2 at $(0, \frac{1}{4}, 0)$

Lattice vectors – Vectors that join lattice pts

– Defn: Any vector which causes (infinite) crystal to be unchanged after translation

(translates with itself)

What are some L.V.s for cube above?

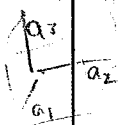
Primitive lattice vectors: (1) the 3 ones (non unique choice) that form basis for all L.V.s

Example: for cube above,

$\vec{a}_1 = (1,0,0)$
$\vec{a}_2 = (0,1,0)$
$\vec{a}_3 = (0,0,1)$

(2) and are as "small as possible" (a consequence of (1), really. See fig 3 pg 5

Small as possible: defined by volume of space of parallelepiped defined by $\vec{a}_1, \vec{a}_2, \vec{a}_3$



$$\text{volume} = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$

any lattice vector $\vec{R} = n\vec{a}_1 + m\vec{a}_2 + l\vec{a}_3$

Basis vectors - vectors from origin to basis atoms
↳ position of lattice point

j atoms: $\vec{r}_j = x_j \vec{a}_1 + y_j \vec{a}_2 + z_j \vec{a}_3$

if desired, can pick origin so

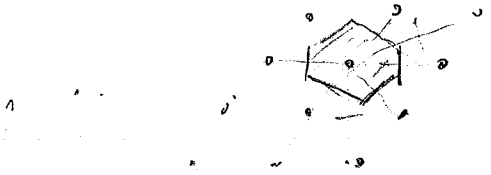
x_j, y_j, z_j all between 0 → 1.

Wigner-Seitz cell

- a "primitive lattice cell" = parallelepiped formed by $\vec{a}_1, \vec{a}_2, \vec{a}_3$

→ How many will there be in a given volume?
Answer: the same as # of lattice pts.

- the WS cell = a specially chosen primitive cell



region enclosed by perpendicular bisectors.

class 1
class 2

primitive basis

- a basis that's based on a set of primitive L.V.s.

Symmetry, again

1) translation (already discussed)

2) rotation — defined by axis about which x'tal can be rotated

simple cubic: 90°, 180°, 270° about x
C_4, C_2, C_4^3
C_2^2

also about y, z

Notation... let's not bother (?)
$\bar{C}_{4x}$ = 270° rotation about x-axis C_{4x}^+ = 90° rotation

3) reflection: defined by plane about which x'tal atoms can be reflected σ_x

4) combo: rotation + reflection labeled "S"

5) inversion: if pt exists through which all atoms can be inverted "I"

group = set symmetries together form a "group"

Symmetry of crystal vs symmetry of lattice