Wed. Oct. 10

- So far we have discovered that the discrete nature of solids leads to properties that would not arise in continuous media

  e.g. • specific heat of solids @ low T
  • non-linearity + branching in the dispersion relations of phonons

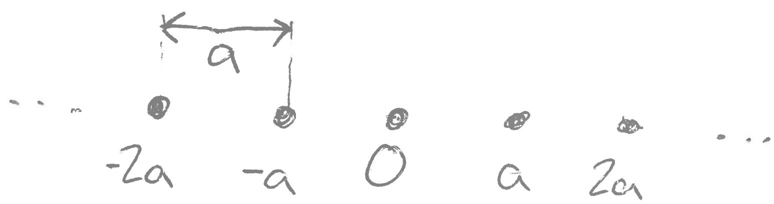
- although we have talked some about bonding in solids arising from electrostatics, we have not spent much time discussing ordering in solids
- often the lowest energy config. is a crystal with periodicity that is regular
- we saw the effect of periodicity for phonons which scatter strongly as $\lambda \to a$, where 'a' is the periodicity of the crystal

- Crystalography is an extensive topic & a critical aspect of the field is that it is independent of the properties of the atoms

* <u>Crystal structure</u>: Some definitions

- lattice: an infinite set of points defined by integer sums of a set of non-colinear lattice vectors

  - We have seen a lattice before in the 1D solid where 'a' is the equilibrium spacing



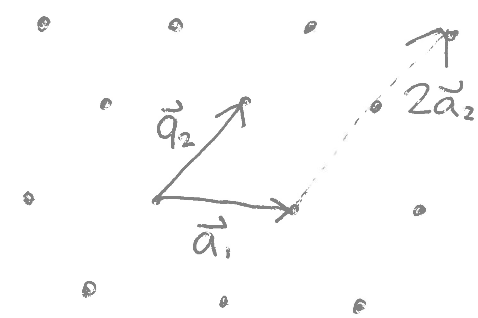
  - the points of the lattice are given by $R = na$ (eq. positions)

  - in 2D, for example

  - points are at location

$$\vec{R}_{[n_1, n_2]} = n_1 \vec{a}_1 + n_2 \vec{a}_2$$

$$n_1, n_2 \in \mathbb{Z}$$



- Without plotting points, we extrapolate to 3D

$$\vec{R}_{[n_1 n_2 n_3]} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

$$n_1, n_2, n_3 \in \mathbb{Z}$$

- Clearly, the addition of any two vectors in the set gives another vector in the set
  $\rightarrow$ translational symmetry

- We have assumed a perfect periodic crystal, which do not exist in nature (even crystal face destroys periodicity)

- Thermal vibrations translate atoms away from lattice points (equilib. positions)

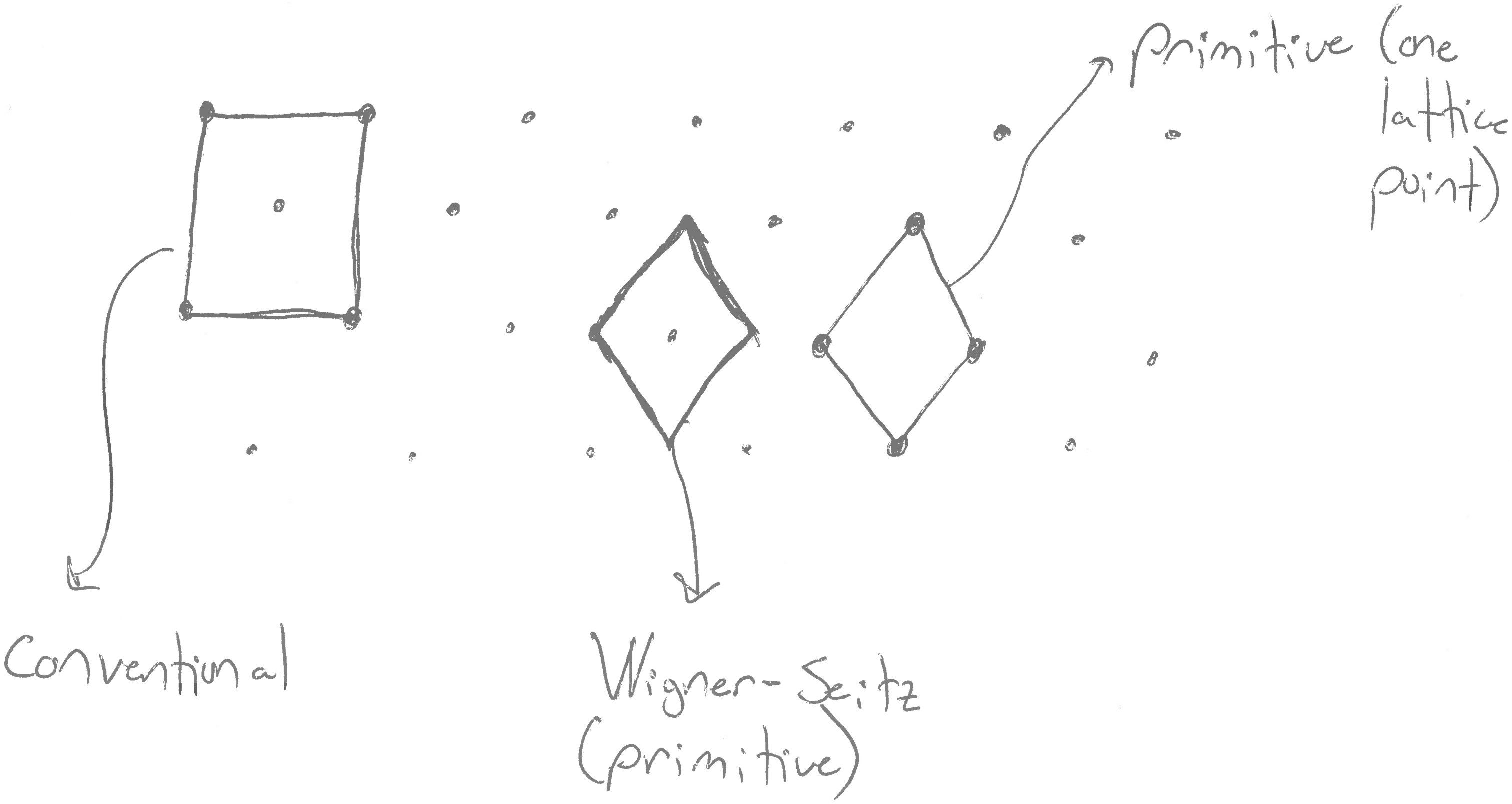
- foreign atoms always present (best technologies $\sim 10^{12}/cm^3$)

- foreign atoms have profond consequences for technologies

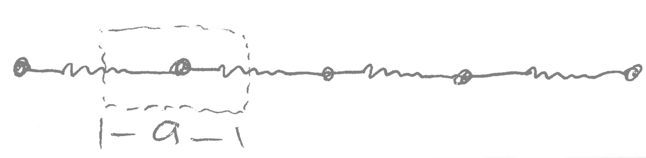
- **The unit cell**: a spatial region with the property that when identical units are "packed" together, it "tiles" and reconstructs the entire cell

- **primitive cell**: only one lattice point in the cell (a unit cell)

- **Unit cells are not unique**

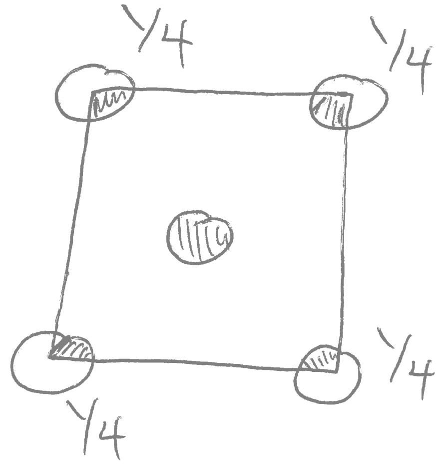


- **Ex**: for 1D case, primitive cell is not unique but must be of length 'a'



$\ast$ Notice something about the # of lattice points in a cell

<u>Ex</u>: conventional



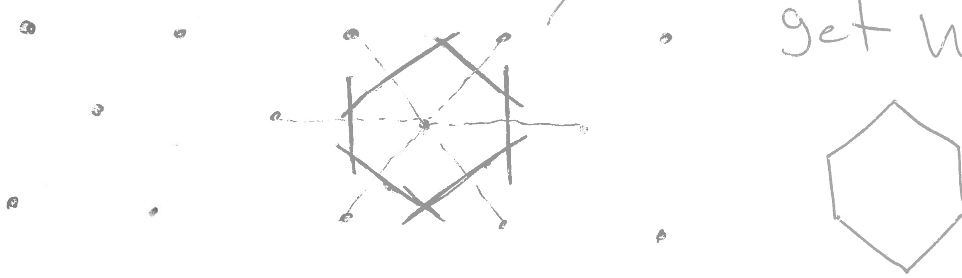
- # points in a cell $= \frac{1}{4}(4) + 1 = 2$

$$\underset{\text{edges}}{\frac{1}{4}(4)} + \underset{\text{center}}{1}$$

- not a primitive cell (2-points)
- for Wigner-Seitz cell, all points in (within lines) space of cell are closer to lattice point than other points
- <u>construction</u>: draw lines to nearest neighbors, then bisect these lines at their midpoints w/ $\perp$ lines

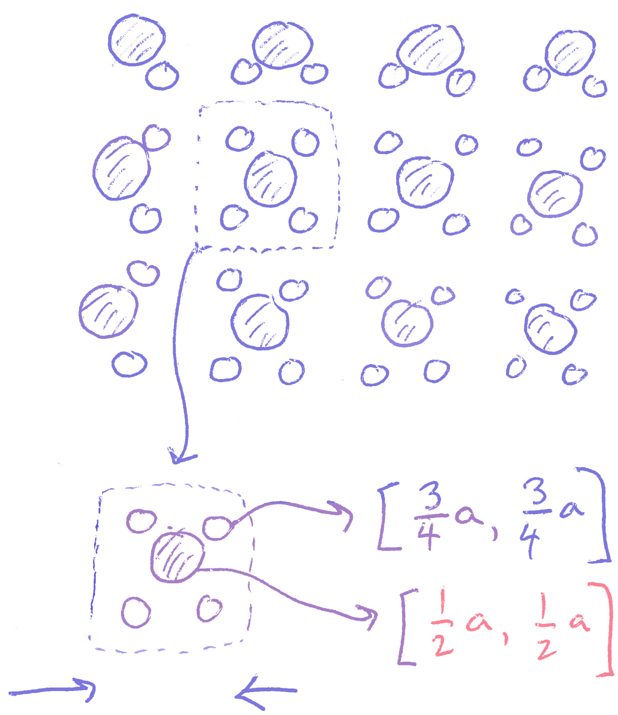
- <u>Ex</u>:

clean lines to get W-S cell



- **Basis:** description of objects within unit cell with respect to the lattice point within cell

Ex:



$\left[\frac{3}{4}a, \frac{3}{4}a\right]$

$\left[\frac{1}{2}a, \frac{1}{2}a\right]$

} locations of atoms in cell

- **Bravais lattice:** all lattice points are equivalent
  - for non-Bravais lattices, the points may be geometrically different or different atoms