The idea of crystals.

The goal of condensed matter physics is to understand how the fundamental laws of nature unfold themselves in objects of the natural world. Because of the complexity of c.m. systems is so enormous, the number of atoms is so great, and the possibility of solving all underlying eqns is so remote, the laws of great importance are principles of symmetry. A first step is to describe how atoms are arranged. The idea of the crystal has emerged out of an obscure class of minerals to dominate thought about all solids.

A small group of atoms repeats a simple pattern endlessly through the stretches of a macroscopic body. The real world does not have perfect crystals, nevertheless the science

of condensed matter physics begins with the crystal, its single most important structural idea.

Why are solids crystalline?

Crystalline order is the simplest way that atoms could possibly be arranged to form a macroscopic solid. Small basic unit of atom repeats endlessly. Why are low-energy arrangements often periodic? If there is some optimal neighborhood for each atom, then the lowest energy state for a large number of atoms gives the same neighborhood to every atom. There is no proof and there is exaption (helium is liquid even at T=0). Equilibrium lattice structure may be a function of temperature and pressure.

(even small oscillations of ions may change the entropy $\Leftarrow$ the energy differences between different crystalline configurations are small $\sim 10^{-4}$)

Two dimensional lattices

2-dim lattices are easier to picture and understand than 3-d. All the central definitions ~~for~~ for lattices will be first introd. in a 2-dim setting.

Bravais lattice

A collection of points in which the neighborhood of each point is the same as the neighborhood of every other point under some translation is called a Bravais lattice.

In 2-dim., the location of every point in such a lattice can be described in the form

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2$$

$\vec{a}_1$ and $\vec{a}_2$ are 2-dim vectors, called the primitive vectors

They must be linearly independent.

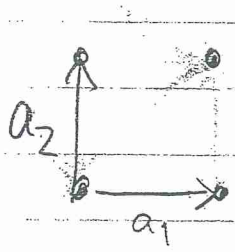
n_1 and n_2 are integers.

Give picture of some Bravais lattice

2 dim Bravais lattices

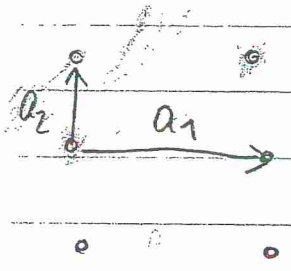
In $d=2$ there are 5 Bravais lattices.

1) Square lattice: symmetric under

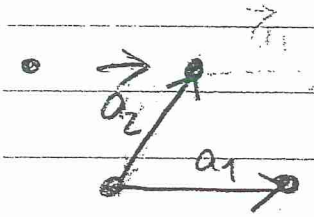


reflection about both x and y and with respect to 90° rotations.

2) Rectangular lattice: ~~so to~~ sq. lat. compressed along one axis. It has no rotational sym (but has a reflection sym.)



3) Hexagonal lattice: invariant under reflections about x and y and rotat by 120°.

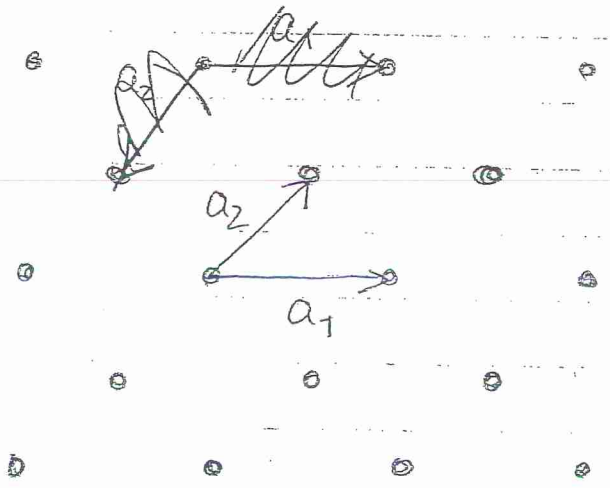


For the hexagonal lattice one can take

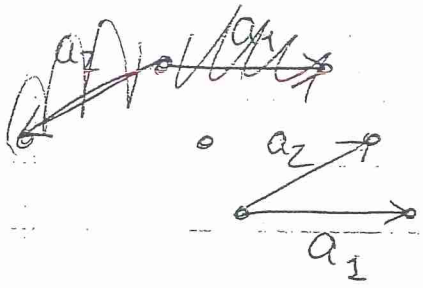
$$\vec{a}_1 = a\,(1, 0)$$

$$\vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$

4) Centered rectangular lattice : it results from compressing the hexagonal lattice (↓ no rotat sym by 120°)



5) Oblique lattice : An arbitrary choice of $\vec{a}_1$ and $\vec{a}_2$ with no symmetry.



The choice of primitive vectors is not unique - one makes choices that are as simple or convenient.

Example for the hexag. lat. we chose

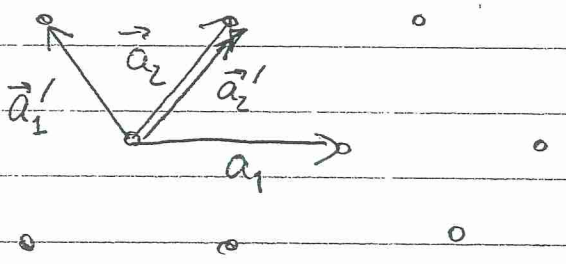
$$\vec{a}_1 = a\,(1,\,0)$$

$$\vec{a}_2 = a\left(\frac{1}{2}\quad\frac{\sqrt{3}}{2}\right)$$

We could also choose

$$\vec{a}_1' = a\left(-\frac{1}{2}\quad\frac{\sqrt{3}}{2}\right)$$

$$\vec{a}_2' = a\left(\frac{1}{2}\quad\frac{\sqrt{3}}{2}\right)$$



The only mistake is to choose a set of vectors ~~that~~ which is not linearly independent.

Lattices with Bases

The neighborhoods of all particles must be identical under translation for a structure to be a Bravais lattice.

Many lattices occuring in nature are not Bravais lattices, but lattices with a basis. Lattices of this type are constructed by beginning with a Bravais lattice, but putting at each lattice site an assembly of particles (rather than 1, the same assembly for each site)

Example: Honeycomb lattice

Start with a hexagonal lattice

$$\vec{a}_1 = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

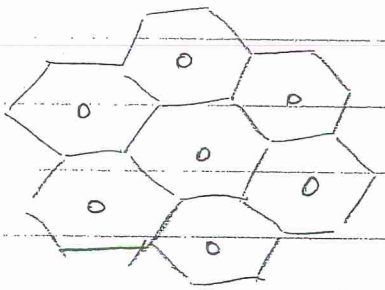
$$\vec{a}_2 = a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$$

Decorate every lattice point with

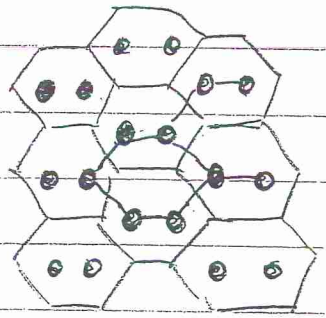
Basis particles at

$$\vec{v}_1 = a\left(\frac{1}{2\sqrt{3}}, 0\right)$$

$$\vec{v}_2 = a\left(-\frac{1}{2\sqrt{3}}, 0\right)$$



Hexagonal lattice

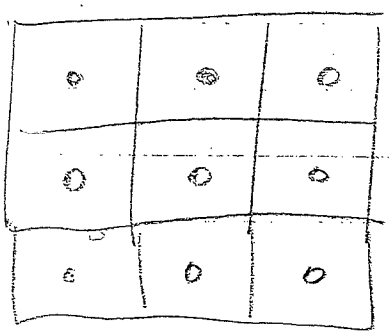


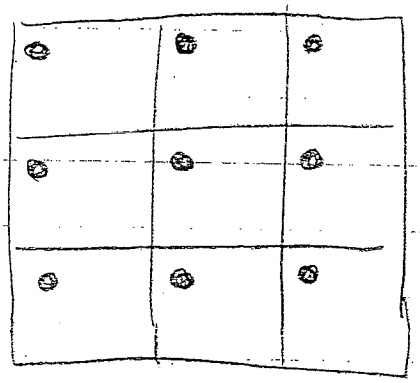
Honeycomb lattice

Primitive Cells

Lattices are created by repeating small basic units. So the full information of a crystal can be contained in a small region of space. Such a region chosen to be as small as it can be, is called a primitive cell.

Primitive cells are not unique:





unit cell can also have funny shape

two primitive cells for a square lattice (particle in the corner or in the center)

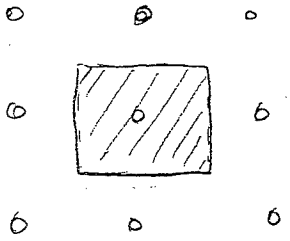
~~However~~ The area of a unit cell is unique: it contains exactly one particle.

Wigner-Seitz Cells

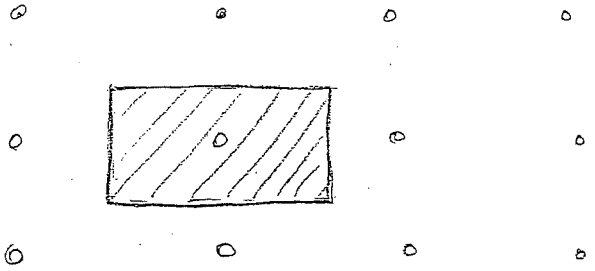
A standard way of constructing a primitive cell that is invariant under all symmetry operations that leave the crystal invariant — Wigner-Seitz cell. With each lattice point associate all of space which is closer to it than any other lattice point. This relation does not change under any operation that leaves the lattice inv. => the W.-S. cell displays the full symmetry of the lattice.

Wigner - seitz cells for the 2 dimensional lattices

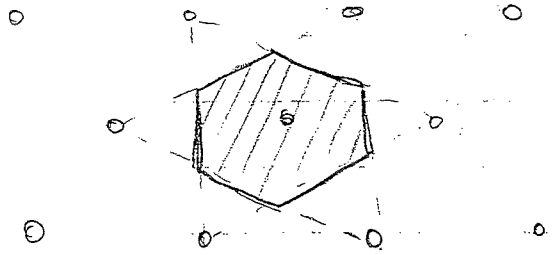
Square



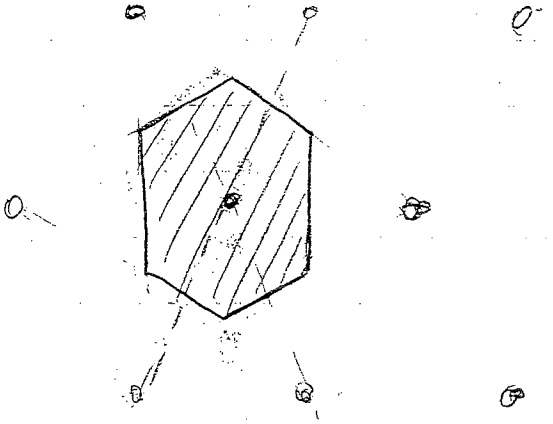
Rectangular



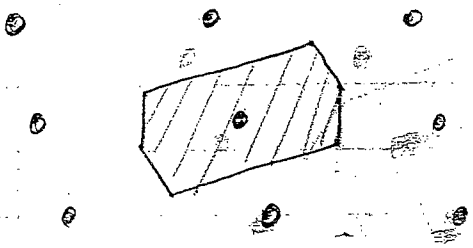
Hexagonal = triangular



Centered rectangular



Oblique



(Ash-Mermin p. 71)

Coordination number

The points in a Bravais lattice that are closest to a given point are called its nearest neighbors. (each point has the same # of near. neighb.) The # of the near. neighb = coordination number. This defin. can be extended to non-Bravais lattices provided that each point in the array has the same # of nearest neighbors.

Examples: coord # of square = 4

hexagonal → 6

honeycomb → 3.