project: I-3

"Basics"

Chapters 1-3 Crystal Structure (Focus on Ions)

1) Description of
2) Expt Measurement (x ray scattering)
3) Bonding - what holds solid together

→ Chapters 19-21 Defects

Chapters 4-5 Crystal Vibrations (Phonons)

Chapters 6-9 Electronic Structure

→ Chapter 17 Surfaces

→ 18 Low D

6) Electrons with no crystal (!)
7) Effect of crystal - energy bands
8) Semiconductors } experimental determination
9) Metals

Chapter 10 Superconductivity

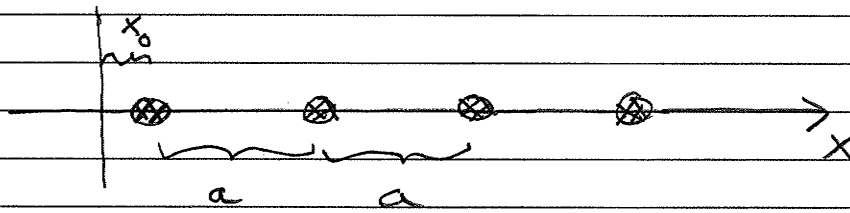
Chapters 11-13 Magnetism

Chapters 14-16 Interaction of Light with Solids

project: I-4

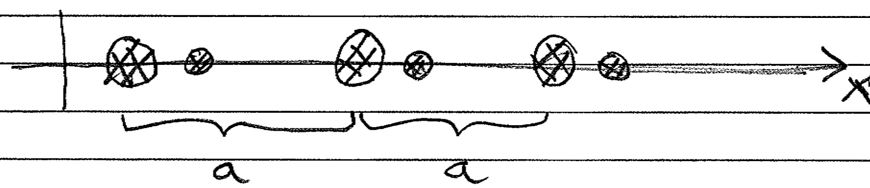
Crystals are periodic arrays of atoms. We will start in low d since easier to draw.

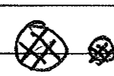
Suppose only one type of atom:



Atoms located at $x_n = x_0 + na$

If more than one type of atom:

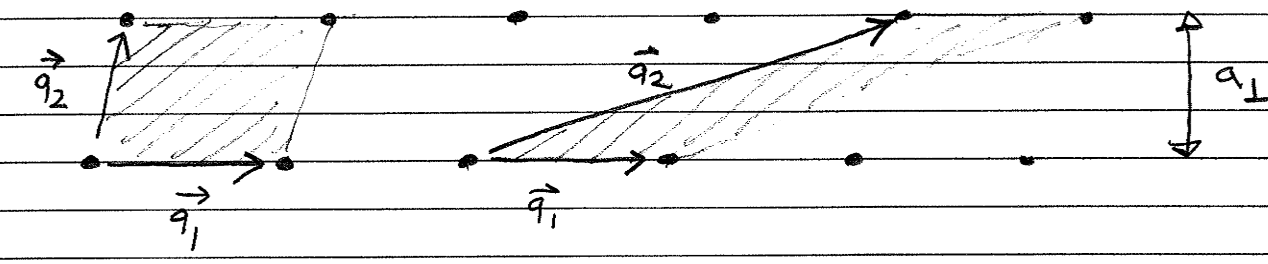


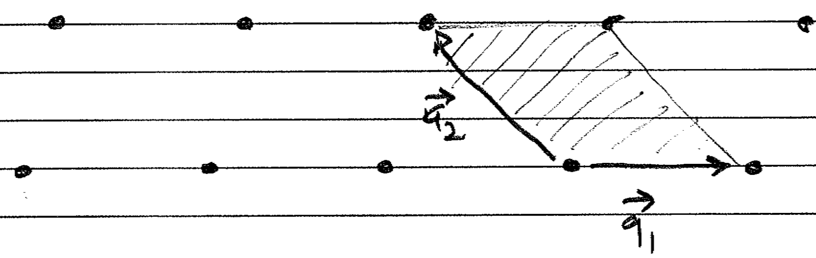
one specifies the separation "a" but also the "basis" ie the collection of atoms  that repeats

Note the lattice looks the same is you look at set of lattice points $x_0 + n(2a)$ or $x_0 + n(3a)$ but the $x_0 + na$ set is said to be <u>primitive</u> because it has the smallest length (area, volume)

project: I-5

In 2d need 2 vectors





There are also many choices of $\vec{q}_1, \vec{q}_2$ which are primitive (smallest area). All choices above have same area $|\vec{a}_1 \times \vec{a}_2|$

WHY? $\quad \vec{q}_1 \times \vec{q}_2 = |\vec{q}_1| \, |\vec{q}_2| \sin\theta_{12}$

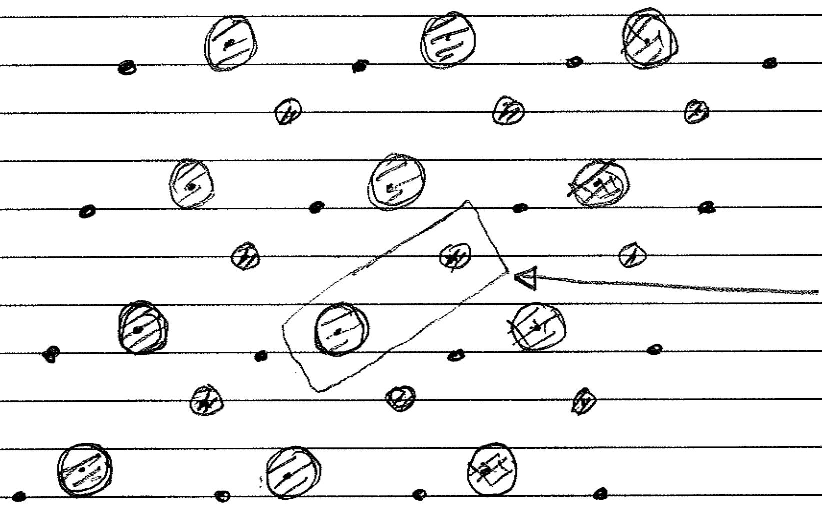
and in pictures above $|\vec{q}_2| \sin\theta_{12} = q_\perp$ is same for all choices

Again, lattice will look the same with some choices of $\vec{q}_1$ and $\vec{q}_2$ with <u>bigger</u> $|\vec{q}_1 \times \vec{q}_2|$ but then we will not call them "primitive"

project:

I-6

Two types of atoms (ie basis) in 2d: An example



basis is this collection of two atoms

They are at $j = 1, 2$

$$\vec{r}_j = x_j \vec{a}_1 + y_j \vec{a}_2$$

$$0 < x_j, y_j < 1$$

relative to lattice point

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

DiVOGA

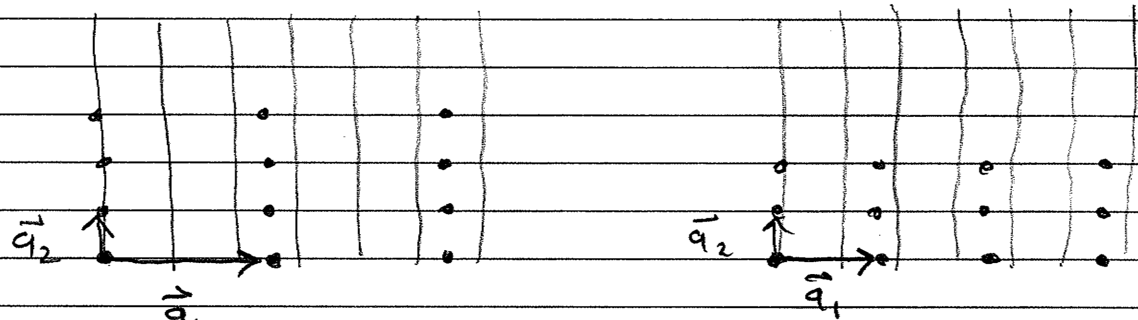
project: I -7

Natural to ask how many "types" of lattice there are.

What do we mean by "type"?

Would you consider lattices with $\vec{a}_1 \perp \vec{a}_2$

and $|\vec{a}_1| = 2.7|\vec{a}_2|$ different from $|\vec{a}_1| = 1.9|\vec{a}_2|$?



$|\vec{a}_1| = 2.7|\vec{a}_2|$ $\qquad\qquad$ $|\vec{a}_1| = 1.9|\vec{a}_2|$

If you say "different" than there are clearly an

∞ # of lattices in 2d corresponding to the ∞ #

of choices of $|\vec{a}_1|/|\vec{a}_2|$

What else could you do?

Instead base definition of type on symmetry.

Lattice which is invariant under rotation by $\pi/2$ must

be a square lattice $\vec{a}_1 \perp a_2$ and $|\vec{a}_1| = |\vec{a}_2|$

"4 fold axis"

project: I-7'

Argument for # lattice types in d=2

set scale of length

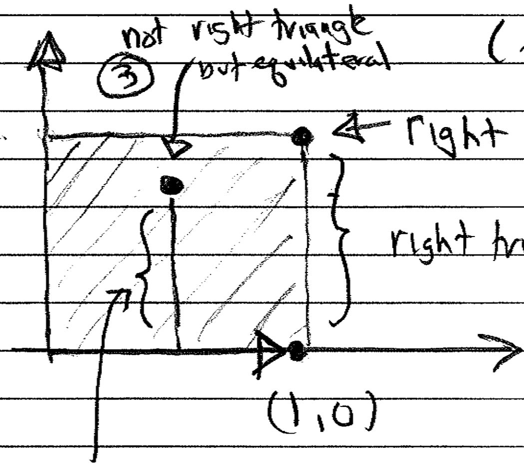
Without loss of generality can choose $\vec{a}_1 = (1,0)$

Then also can choose $\vec{a}_2 = (x,y)$ with $y>0$

$x<1$

make $\vec{a}_1$ be the longer of 2 vectors

Now ask what special (x,y) there are (from symmetry point of view)



right triangle (isosceles) ①

right triangle (not isosceles) ②

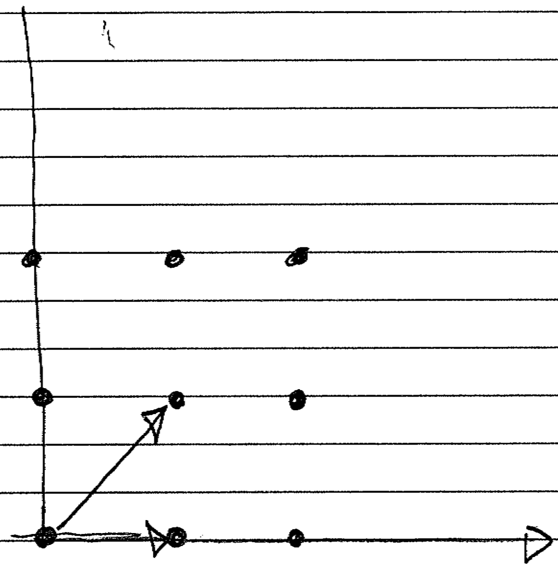
there is also a right triangle isosceles on this path but equivalent to ① in symmetry sense

not right triangle, not equilateral but isosceles ④

⑤ anything else

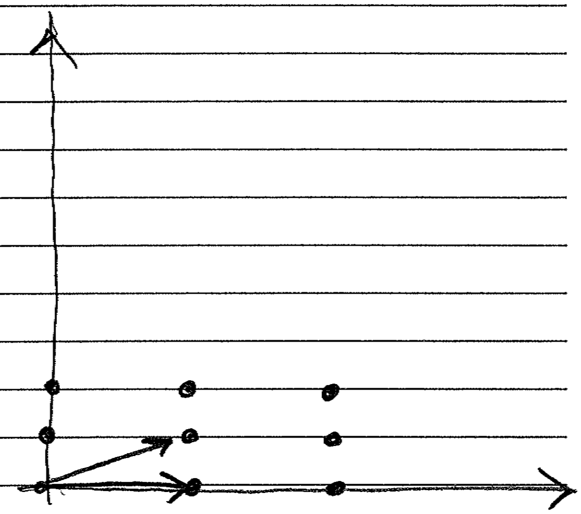
project: I-7"

① Right triangle, isosceles



gives square lattice

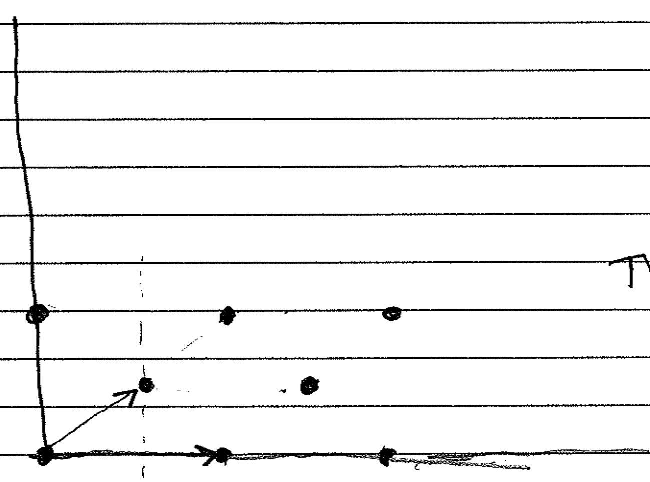
② right triangle, not isosceles



gives rectangular lattice

③ equilateral → hexagonal lattice (obviously)

④ not right triangle, not equilateral, but isosceles



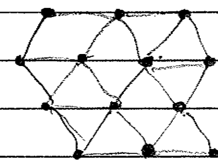
This is Kittel's "rectangular centered"

project:

I-8

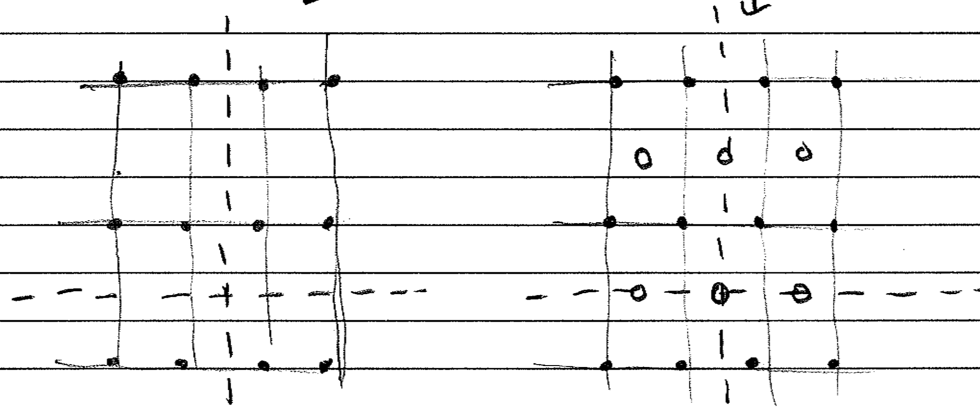
3 fold axis : hexagonal

(rotation by 120°)



2 mirror planes : rectangular primitive

or rectangular centered



There are only these 4 special types and then the general "oblique" lattice which has no special symmetry.

DiVOGA

project:

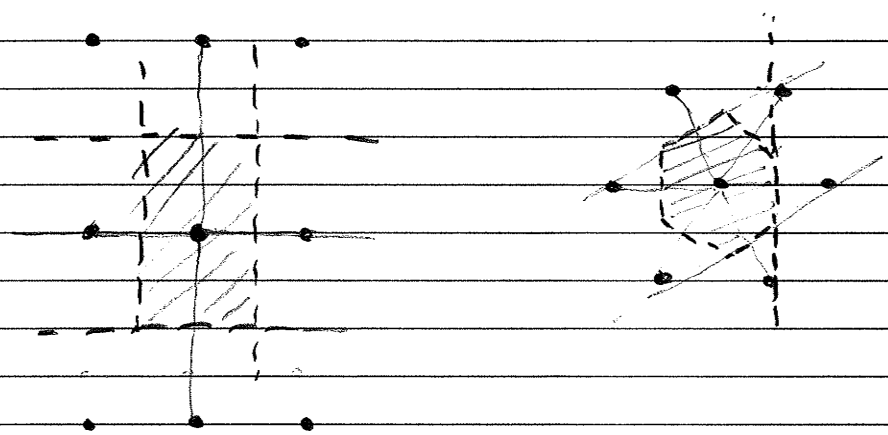
I - 9

On page I-5 drew some possible primitive cells.

The "Wigner-Seitz" cell is an interesting one formed (in $d=2$)

by choosing $\perp$ bisectors of segments connecting lattice point

to its neighbors



In $d=2$ volume of primitive cell is $|\vec{a}_1 \times \vec{a}_2| = V$

In $d=3$ it is $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = V$

Can you think of some examples / special cases

which fit in with this formula (eg $\vec{a}_1$ is in

the same plane as $\vec{a}_2$ and $\vec{a}_3$ what is V ?)