Physics 410/510 – Solid State Physics
Spring 2015
Monday, week 1:

- What is Condensed Matter Physics?
  - Largest single subfield of physics
  - Practical → Abstract

- Why study Condensed Matter?

  (1) It is all around us. We may ask:

  i) Why are metals shiny?

  ii) " cold?

  iii) Why is glass transparent?

  iv) Why is water fluid & wet?

  v) Why is rubber soft & stretchy?

  (2) It's Useful

  i) New materials

  ii) Semiconductor Technology → Electronics

  (3) Deep & Important Physics

  i) Over 50 Nobel prizes

  ii) Anderson-Higgs mechanism same as Higgs in HET, described first by Anderson working w/ Semiconductors.

  iii) Renormalization Group (Ken Wilson) developed simultaneously in CMT & HET.

  iv) Topological QFT dev. by string theory, discovered in CM Lab.

  v) String theorists applying Black-Hole Physics to phase transitions

(4) Reductionism doesn't work

- Understand microscopic theory, but macroscopic properties emerge that we did not expect.
- Asking "What is it made of" doesn't always tell us why something is the way it is. For example, we will need to solve the Schrödinger equation to understand water, but it is impossible.

(5) CM is the best lab we have for studying Quantum & Statistical Mechanics.

- Why Solid State?
  - Biggest single subfield of CM
  - Most successful & technologically useful subfield.
    - "Solid" state" Electronics
    - Solids are important industrially
  - Foundational for other CM & other physics.

- Introductions
- Course information:
  - Hand out syllabus.
  - Note about prerequisites:
    - E&M, Mechanics, Stat. Mech, & Quantum highly recommended.
    - I encourage you to continue with the course, but it's ok to wait until you have background.
  - Kittel
  - HW → Biweekly, Thursday by 7 p.m. + Cite
  - Two GTFs + Grad, Ugrad : Will grade Ugrad equately.

- Course Project:
  - Choose something that you would like to explore in more detail:
    - Topological insulators
    - Majorana Fermions
    - Superconducting Qubits

  or, do an experiment (build a transistor or LED), or explain how some solid state device works (MOSFET, etc.), or make note cards.

- Schedule → See it for reading. We may not get to Fermi Surfaces & Superconductivity.
- BTW: Next year we'll have 2 Quarters!!
- Website!! HW, Forum, additional reading & lecture notes & Announcements.

The structure of Materials:

Matter (& Solids!) is composed of atoms, which behave quantum mechanically. Attempts to describe the properties of solids w/o Quantum have invariably fallen short, sometimes in drastic ways (e.g. w/ semiconductors, metals, insulators, & the bandgap.)

We will get a lot by observing how atoms or electrons interact with a periodic structure in crystalline solids, so it will be important to review some basic atomic physics & chemistry.

The Periodic Table:

- Chemistry, Atoms, & the Schrödinger Equation

In a sense, asking about how atoms stick together in molecules or in solids is trying to solve the Schrödinger Equation:

wave function

$$H\psi = E\psi \qquad (1)$$

Energy

$H = K.E. + P.E.$

- p_i, r_i, R_i are operators!

$$\underbrace{\sum_i \frac{p_i^2}{2m_i} + \sum_j \frac{P_j^2}{2M_j}}_{K.E.} + \underbrace{\frac{1}{2}\frac{1}{4\pi\epsilon_0}\sum_{j',j} \frac{Z_j Z_{j'} e^2}{|\vec{R}_j - \vec{R}_{j'}|}}_{\text{Nuclei - Nuclei}}$$

$$\underbrace{-\frac{1}{4\pi\epsilon_0}\sum_{j,i} \frac{Z_j e^2}{|\vec{r}_i - \vec{R}_j|}}_{\text{electron - Nuclei}} + \underbrace{\frac{1}{2}\cdot\frac{1}{4\pi\epsilon_0}\sum \frac{e^2}{|\vec{r}_i - \vec{r}_j|}}_{\text{electron - electron}}$$

(This is the $\vec{F}(\vec{r},\vec{v},t) = m\, d^2\vec{r}/dt^2$ of quantum objects)

Solving (1) for more than a few particles is impossible. This reductionism isn't helpful, so we need some simple models to learn about what is going on.

- Structure of Periodic Table

  - Fundamentals of electrons in isolated atoms

$$|\psi\rangle = |n, l, l_z, \sigma_z\rangle \qquad \text{where}$$

principal Quantum #

$n = 1, 2, \ldots$

$l = 0, 1, \cdots, n-1$

angular momentum

$l_z = -l, \cdots, l$

z-component

$\sigma_z = +\frac{1}{2}, -\frac{1}{2}$

z-comp. of spin

Recall,

$l = 0, 1, 2, 3, \ldots$

s p d f

↓

in atomic language these are "shells"

useful mnemonic

(smart physicists don't find giraffes hiding)

s p d f g h

The $l = 0, 1, 2, 3$ shells can have # electrons $= 2, 6, 10, 14$

$2 \times (2l + 1)$

spin ↑↓ # l_z state

How do electrons fill up shells or states?

- <u>Aufbau ("build up") Principle</u>: Shells should be filled starting with the lowest available energy state. An entire shell is filled before another shell is started.

- <u>Madelung's Rule</u>: The energy ordering is from the lowest value of $N + l$ to the largest; & when two shells have the same value of $n + l$, fill the one w/ smaller n first.

* PPT of mnemonic.

Although there are few exceptions to the filling rules (e.g. Cu), the periodic table structure is determined by it:

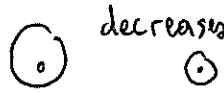
He	Ne
$1s^2$	$1s^2\,2s^2\,2p^6$

- <u>Periodic Trends:</u> (1869 Dmitri Mendeleev)
  - Elements w/ similar chemistry in same column: ↗ determined by outer most shell electrons!

    C, Si, Ge each have $2e^-$ in partially filled p-shell.
    $2p^2\ 3p^2\ 4p^2$

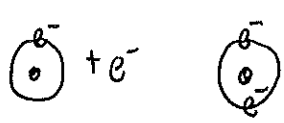
  - <u>Chemical trends:</u>

Atomic Radius ⟶
decreases



Ionization Energy ⟶
Increases

Electron Affinity ⟶
Increases



Electronegativity ⟶
"Tendency to attract e^-"

Physics 410-510 — Solid State Physics
Spring 2015
Wednesday, week 1:

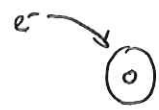
Basic Atomic Physics & Chemistry:

$$|\psi\rangle = |n, l, l_z, \sigma_z\rangle$$

- Colums in periodic table have similar chemistry
- Other trends:

Atomic Radius decreases $\longrightarrow$

Electron Affinity Increases $\longrightarrow$
(Up to Noble Gases)



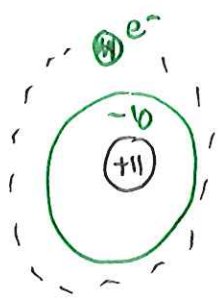
Ionization Energy Increases $\longrightarrow$

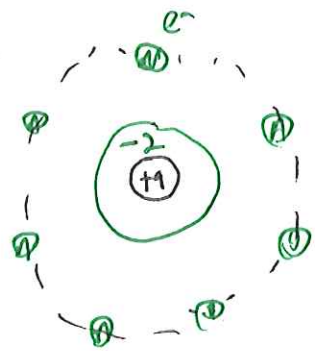
These trends can be understood by looking at the effective nuclear charge.

Effective Nuclear Charge

Electron shielding affects the chemistry & observed trends

Na	Fluorine
11 electrons	9 electrons
1 e^- in 3s	7 e^- in outer most $n=2$ shells





Electron sees little charge... weakly bound.

Electrons see more charge @ Nucleus

What Holds Solids Together? Chemical Bonding:

Ionic, covalent, Van der Waals, dipole, metallic, H-bonds

Ionic: In some compounds, an electron is transferred from one atom to another & the resulting ions attract:

$$A + B \rightarrow A^+ + B^- \rightarrow A \cdot B$$

$$Na \quad Cl \qquad Na^+ + Cl^- \qquad NaCl$$

$$\Delta E_{A+B \to AB} = (\text{Ionization Energy})_A - (\text{Electron Affinity})_B - (\text{Cohesive Energy})_{AB}$$

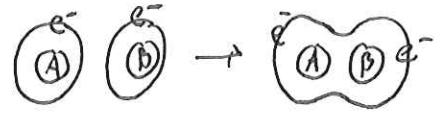
N.B. Electronegativity $= \frac{\text{El. Aff.} + \text{Ionization}}{2}$

Properties:

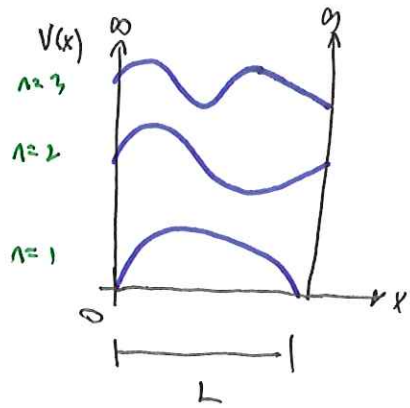
- Hard, very brittle
- High melting T
- Electrical Insulator
- H_2O soluble

Covalent Bond:

Electrons are shared between two atoms



- Particle in a Box:



$$H\psi = E\psi$$

$$H = \frac{p^2}{2m} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$\Rightarrow \quad \frac{d^2\psi}{dx^2} = -\left(\frac{2m \cdot E}{\hbar^2}\right)\psi$$

$$= -k^2\psi \qquad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

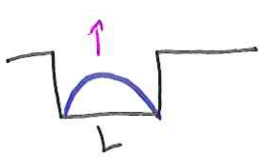
$$\psi(x) = A\cos(kx) + B\sin(kx)$$

- $\psi(0) = 0 \quad \Rightarrow \quad A = 0$
- $\psi(L) = 0 \quad \Rightarrow \quad k \cdot L = \pi \cdot n \qquad n \in \mathbb{Z}^+$

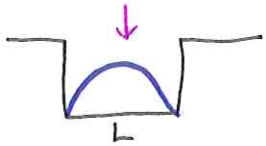
$$\boxed{k_n = \frac{\pi \cdot n}{L}}$$

so $$\boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2} \cdot n^2}$$

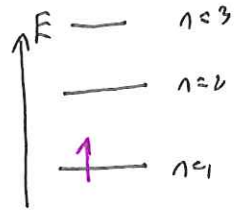
Each electron has:

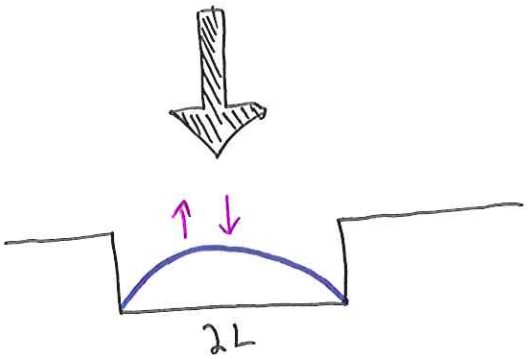


$$E = \frac{\hbar^2 \pi^2}{2mL^2}$$

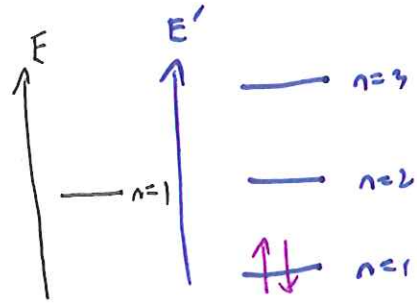


$$E = \frac{\hbar^2 \pi^2}{2mL^2}$$



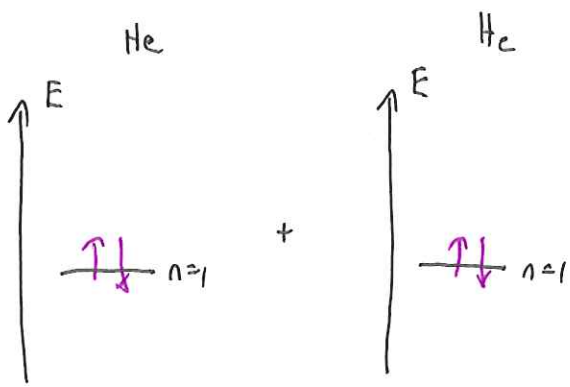


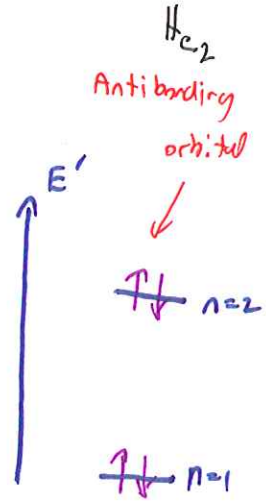
$$\boxed{E' = \frac{\hbar^2 \pi^2}{2m4L^2} = \frac{1}{4} E}$$



This leads to bonding & the $|\psi_n'\rangle$ state is a "bonding" orbital. Note that each "atom" only had 1 e^-.

Now for He

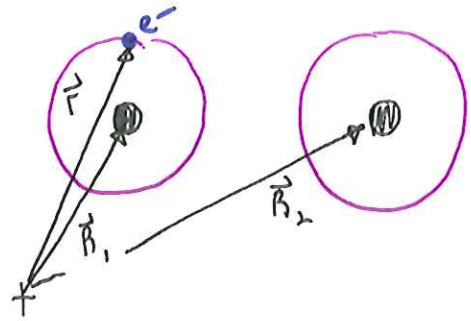




So He_2 doesn't form.

- <u>Molecular Orbital or Tight Binding Theory:</u>

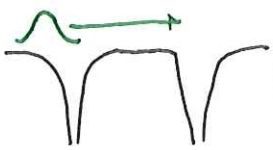
Two Hydrogen atoms



Assume Nuclei are fixed & solve for electronic wavefunction (Born-Oppenheimer approximation) w/ the Hamiltonian

$$H = \frac{p^2}{2m} + V_1 + V_2$$

$$\text{where} \quad V_i = \frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{|\vec{r} - \vec{R}_i|}$$



Here we are solving for <u>1 electron</u> in a potential of <u>2 Nuclei</u>.

We'll use the <u>variation approach</u>:

Let $|\psi\rangle$ be any arbitrary wavefunction & write in terms of eigenfunctions of H:

$$H|n\rangle = E_n|n\rangle$$

$$|\psi\rangle = \sum C_n|n\rangle \qquad \text{w/} \quad \langle\psi|\psi\rangle = \sum_n |C_n|^2 = 1$$

Then

$$\langle\psi|H|\psi\rangle = \sum_{m,n} C_m^* \langle m| H C_n |n\rangle$$

orthogonal

$$= \sum_{m,n} C_m^* C_n E_n \langle m|n\rangle$$

$$= \sum_n |C_n|^2 E_n \geq E_0 \sum_n |C_n|^2 = E_0$$

So $\langle\psi|H|\psi\rangle$ gives an upper bound of ground state energy.

Normally, we take $|\psi\rangle = |\psi(\alpha)\rangle$, then

$$\langle\psi|H|\psi\rangle = E(\alpha)$$

& we minimize $E(\alpha)$, $\frac{dE}{d\alpha} = 0$ to find lowest upper bound of true ground state energy.

Now, guess

"atomic" orbitals or "tight binding" orbitals

$$|\psi\rangle = \phi_1 |1\rangle + \phi_2 |2\rangle \rightarrow \underline{\underline{\text{LCAO}}}$$

Variational parameters

$|1\rangle$ & $|2\rangle$ are groundstates of Sö when only one nucleus is present.

$$\left(\frac{p^2}{2m} + V_1\right)|1\rangle = E_0 |1\rangle$$

$$\left(\frac{p^2}{2m} + V_2\right)|2\rangle = E_0 |2\rangle$$

And assume $\underline{\langle 1|2\rangle = 0}$. Then the variational approach gives

$$\sum_j H_{ij}\phi_j = E\phi_i$$

where $H_{ij} = \langle i|H|j\rangle$

$$H_{11} = \langle 1|H|1\rangle = \langle 1|\frac{p^2}{2m} + V_1 + V_2|1\rangle = E_0 + \langle 1|V_2|1\rangle$$
$$= E_0 + V_{cross}$$

$$H_{22} = E_0 + V_{cross}$$

$$H_{12} = \langle 1 | \frac{p^2}{2m} + V_1 + V_2 | 2 \rangle$$
$$= E_0 \langle 1 | 2 \rangle + \langle 1 | V_1 | 2 \rangle$$
$$= \langle 1 | V_1 | 2 \rangle$$
$$= -t$$

$$H_{21} = \langle 2 | V_1 | 1 \rangle$$
$$= -t^*$$

Then

$$\begin{pmatrix} E_0 + V_{cross} & -t \\ -t^* & E_0 + V_{cross} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = E \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$$

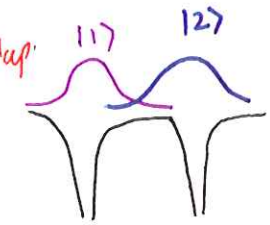
Lead to transition probabilities between $|1\rangle$ & $|2\rangle$

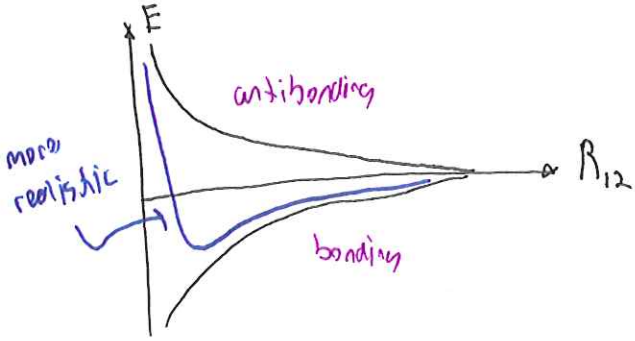
&

$$\boxed{E_\pm = E_0 + V_{cross} \pm |t|}$$

depends on overlap

Interaction w/ second nucleus

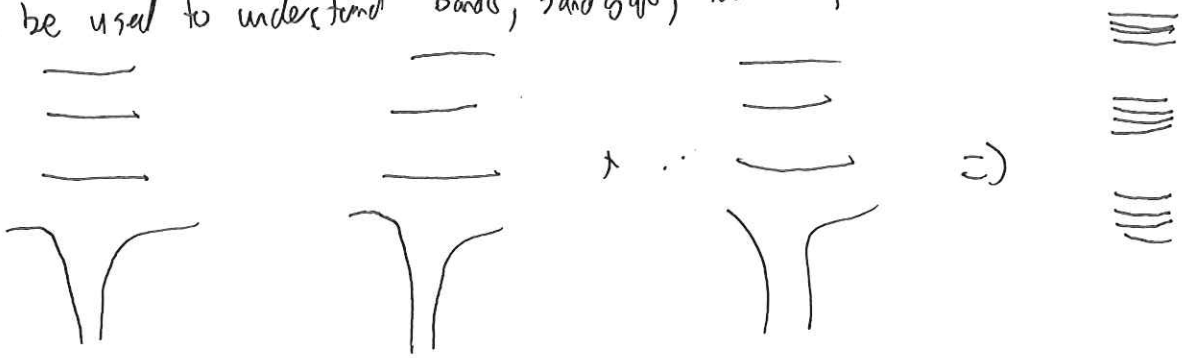




Prop:

- Very hard
- High melting point
- Electrical insulator or semiconductor

Can be used to understand bands, bandgaps, metals & insulators

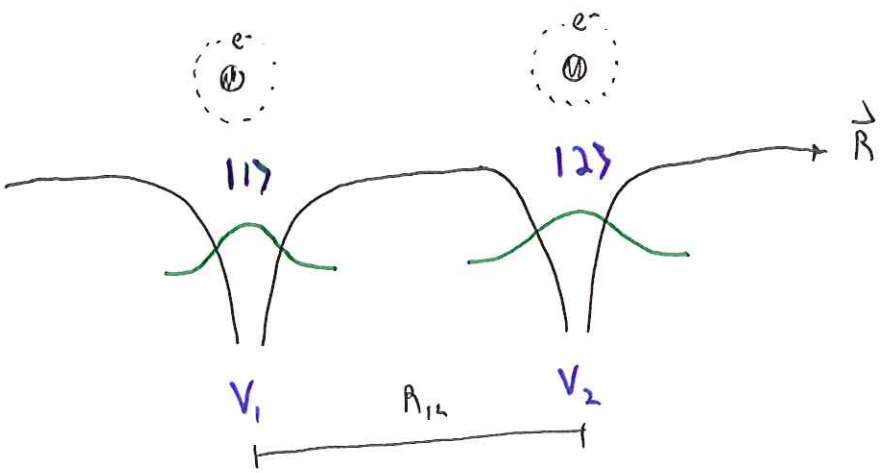


Physics 410/510 — Solid State Physics
Spring 2015
Friday, Week 1:

Review: What holds things together? (Ionic, covalent, dipolar, etc.)

- **Covalent Bonding:**

$$E_0 = \frac{\hbar^2 \pi^2}{2m} \cdot \frac{1}{L^2} \qquad E_0' = \frac{1}{4} E_0$$



Ritz Variational Principle: For arbitrary $|\psi\rangle$, $\langle\psi|H|\psi\rangle = E(\lambda) \leq E_0$

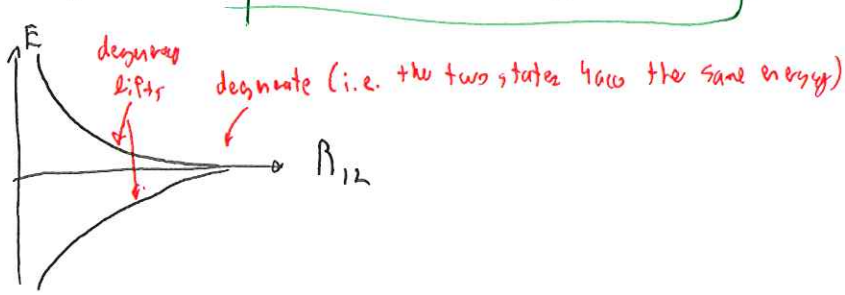
variational parameter

true ground state of H.

variational parameters

$$|\psi\rangle = \phi_1 |1\rangle + \phi_2 |2\rangle$$

$$\sum_j H_{ij} \phi_j = E \phi_i \quad \Rightarrow \quad \boxed{E_\pm = E_0 + V_{cross} \pm |t|}$$

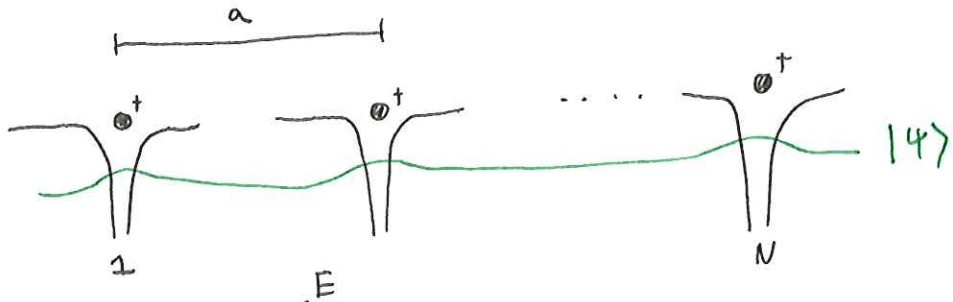


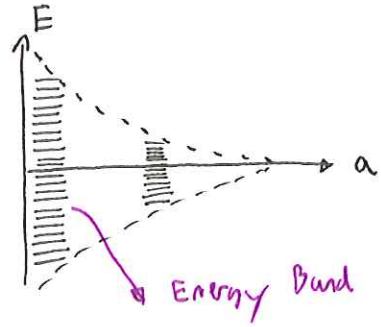
We want to look at crystals where many atoms are bonded together in some sort of periodic arrangement.

★ Show PPT on different crystals

- Ionic (NaCl)
- Molecular (C_{60})
- Polymeric
- Photonic / Phononic artificial xtals
- Liquid

From our tight binding model we see:





Here the periodicity of atoms w/ spacing a leads to lifting of N-degenerate energy levels into bands.

- Crystal structure plays a vital role in determining the properties of solids.

★ PPT of Carbon Crystals

All made of carbon, with markedly different properties.

We will need the language & tools of crystal structure.

Crystal Structure:

• Lattices & Unit Cells

A lattice is:

i) an infinite set of points defined by integer sums of a set of linearly independent primitive lattice vectors

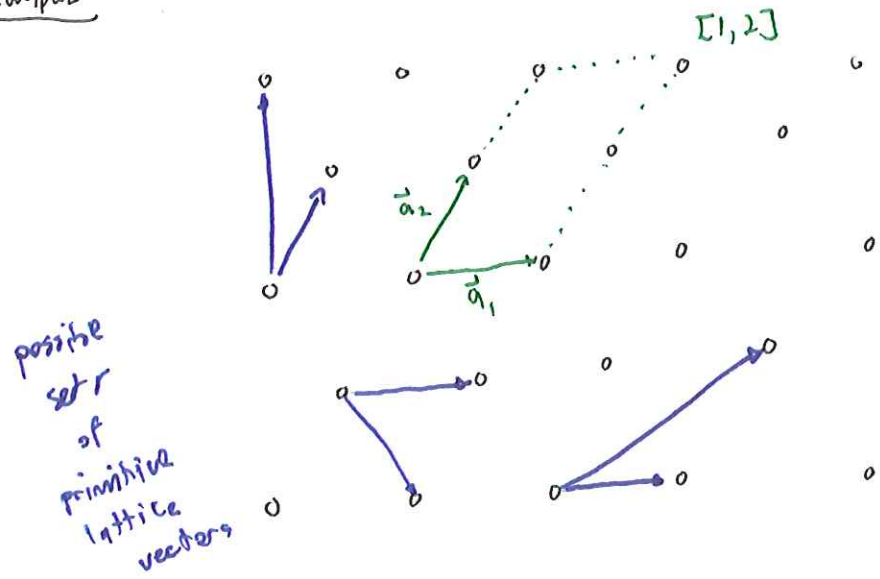
$$\vec{R}(n_1, n_2, n_3) = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$
$$= [n_1, n_2, n_3]$$
$$n_i \in \mathbb{Z}$$

$\vec{a}_i$ primitive lattice vector (Not unique for a lattice)

ii) an infinite set of vectors where adding any two vectors in the set gives a third vector in the set.

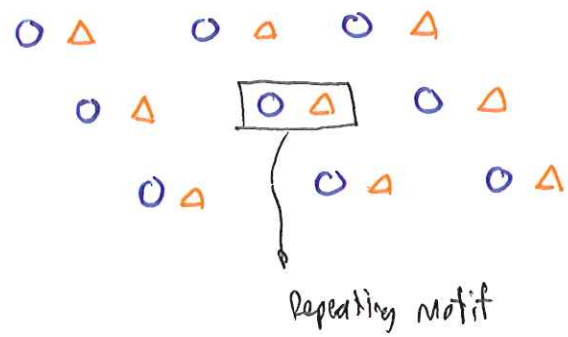
iii) a set of points where the environment looks the same at any point. $\vec{R}' = \vec{R} + [n_1, n_2, n_3]$ for some $[n_1, n_2, n_3]$

Example



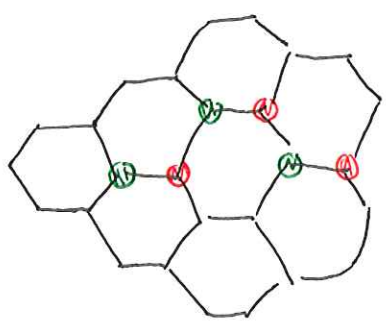
Any periodic structure can be expressed as a lattice of repeating motif

* Show PET of :



N.B. Not all periodic arrangements of points are lattices.

* Show Example of Honeycomb Structure.



A & B dont have same environment.

But this honeycomb pattern is still periodic with a repeating motif, namely,

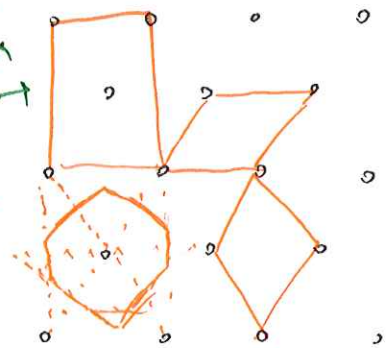
The repeating motif is known as the unit cell.

A unit cell is a region of space (area, volume) that when stacked together with identical units, ~~the full structure~~ it completely fills in or reconstructs the full structure.

Equivalently, a unit cell is the repeated motif which is the building block of the periodic structure.

Q 17: Show unit cells in triangular lattice

often times, rectangular or square unit cells are chosen for their simplicity. → we see this w/ bcc, fcc lattices in 3D.

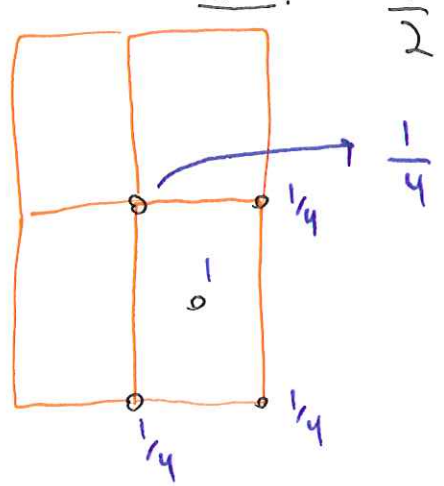


These are all unit cells. Notice that they all reproduce the entire structure. Also, notice that some are smaller/larger than others & so can have different #'s of lattice points.

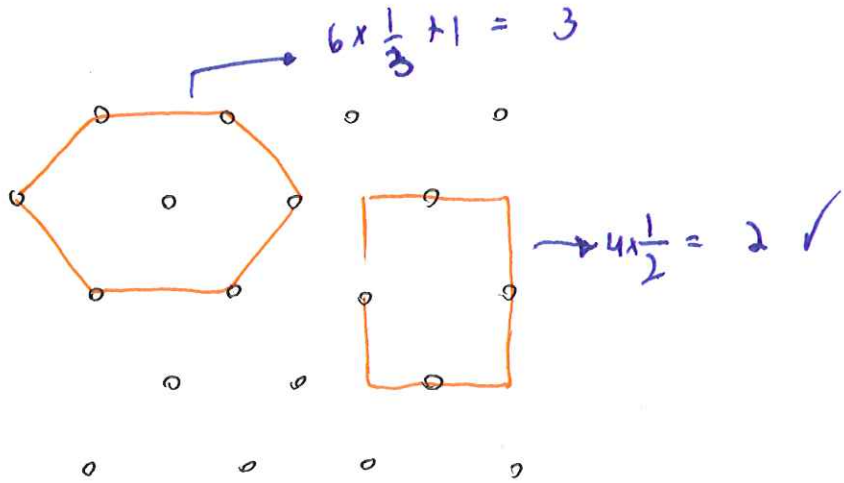
<u>Counting lattice points in unit cells:</u>

- Lattice points are counted fractionally if intersecting numerous cells
  - <u>Corners</u>: $\frac{1}{N}$ $N =$ # vertices meeting at corner
  - <u>Sides</u>: $\frac{1}{2}$

Ex

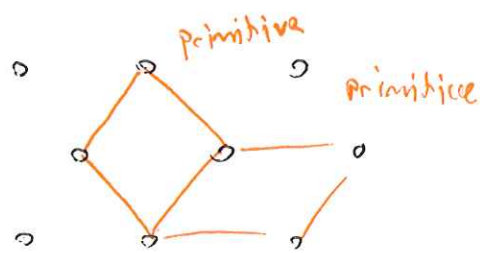


lattice points $= 4 \times (1/4) + 1$
$= 2$



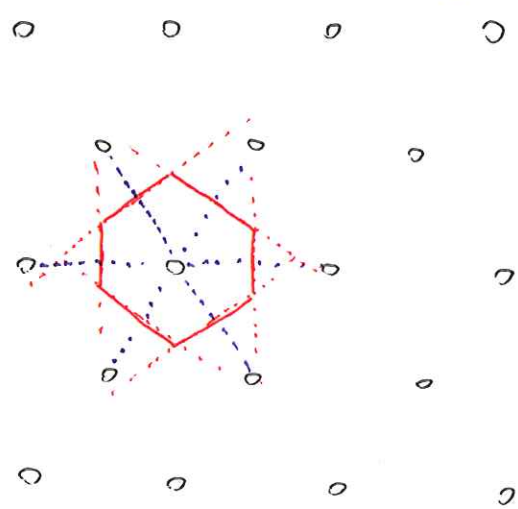
Unit cells containing just 1 lattice point are called primitive unit cell.

Primitive unit cells have the fewest possible # of lattice points (1) & "volume" or "Area."



A special primitive cell is the Wigner-Seitz Cell:

For a lattice point, the volume bounded by the perpendicular direction of nearest neighbors is known as the Wigner-Seitz Cell.



How do we describe periodic structures that are not lattices?

E.g. the honeycomb?

We associate a basis w/ ~~the~~ a lattice.

We call the points of the repeating motif a basis.

The atoms of a basis are referred to the reference lattice point of the unit cell.

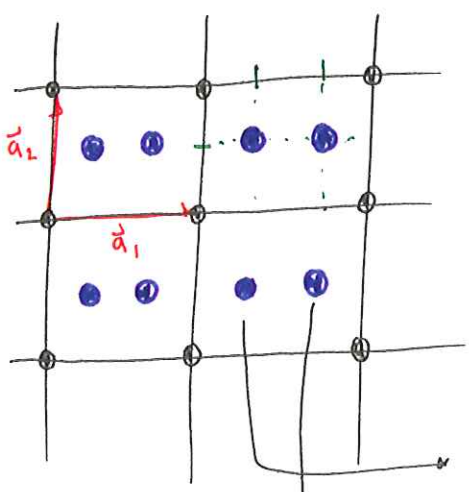
Thus it is said that a crystal (or a periodic structure) is a:

$$\text{Lattice} + \text{Basis}$$

DOI Example: • Honeycomb: 2 atom basis + a Hexagonal lattice

•

Example of Basis atoms in terms of primitive lattice vectors:



$$\vec{B}_{left} = \frac{1}{3}\vec{a}_1 + \frac{1}{2}\vec{a}_2 = [1/3, 1/2]$$

$$\vec{B}_{right} = \frac{2}{3}\vec{a}_1 + \frac{1}{2}\vec{a}_2 = [2/3, 1/2]$$

Later we'll see that a wave gets diffracted by lattice but the intensity of diffraction pattern is determined by the basis.