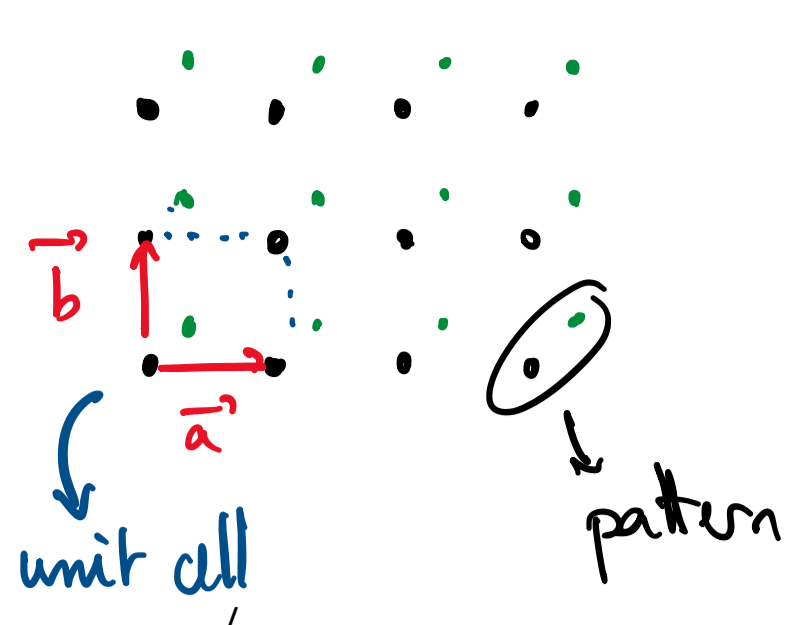


# Reminder: Crystal lattice, Metal bonds

## ① Real and Reciprocal Lattices.



lattice = periodic arrangement of atoms

$$\vec{R}_{uvw} = u\vec{a} + v\vec{b} + w\vec{c}$$

\* Real space  $u, v, w \in \mathbb{Z}$

### Reciprocal space:

Fourier (conjugate) space of the real space

$$\vec{G}_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

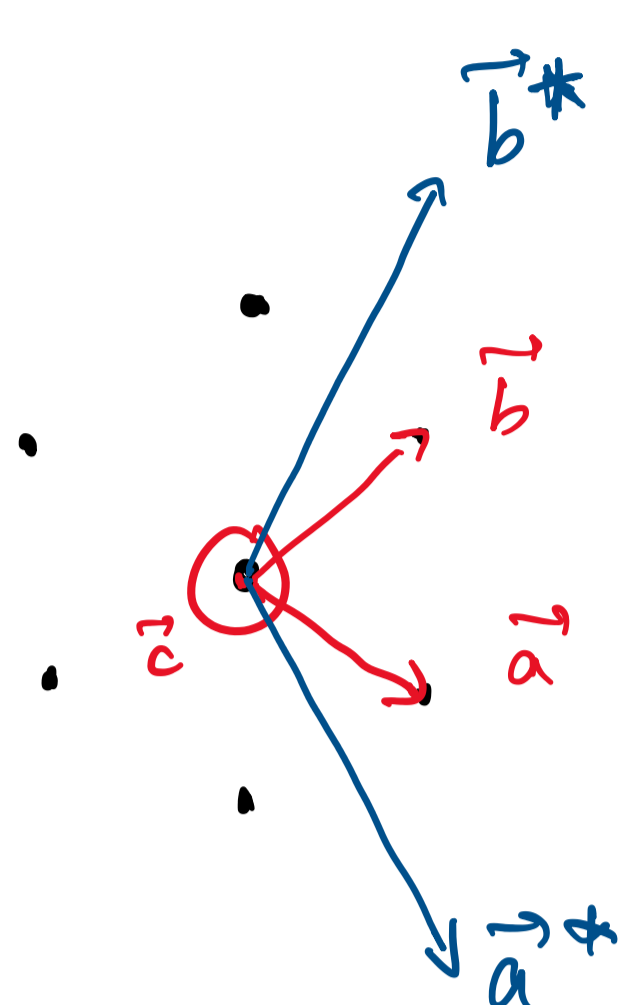
$$\text{with } \vec{a} \cdot \vec{a}^* = \vec{b} \cdot \vec{b}^* = \vec{c} \cdot \vec{c}^* = 2\pi$$

$$\text{and } \vec{b} \cdot \vec{a}^* = \vec{c} \cdot \vec{a}^* = 0$$

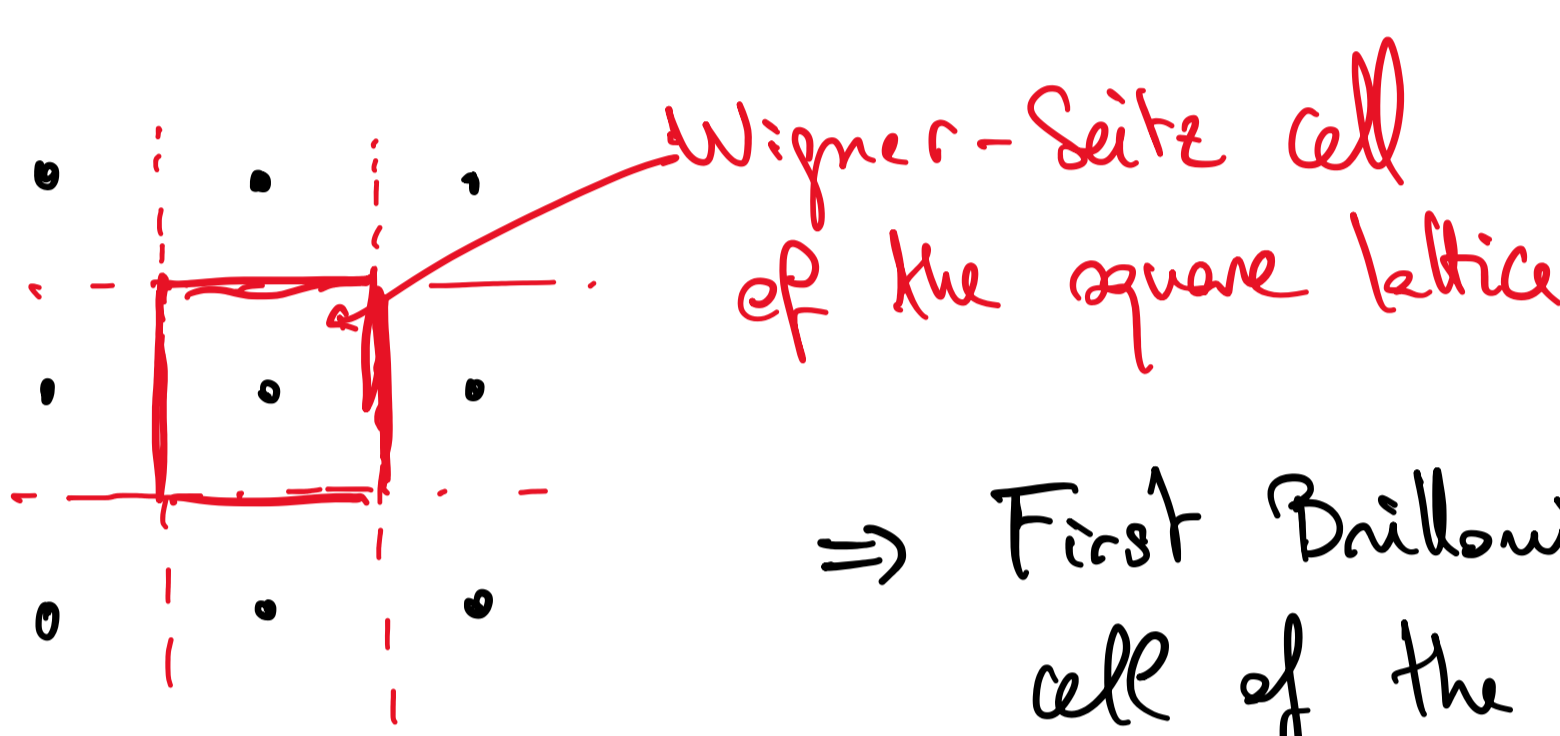
$$\Leftrightarrow \vec{a}^* = (\vec{b} \times \vec{c}) \cdot \frac{2\pi}{V} \quad \text{unit cell Volume}$$

$$\vec{b}^* = (\vec{c} \times \vec{a}) \cdot \frac{2\pi}{V}$$

$$\vec{c}^* = (\vec{a} \times \vec{b}) \cdot \frac{2\pi}{V}$$

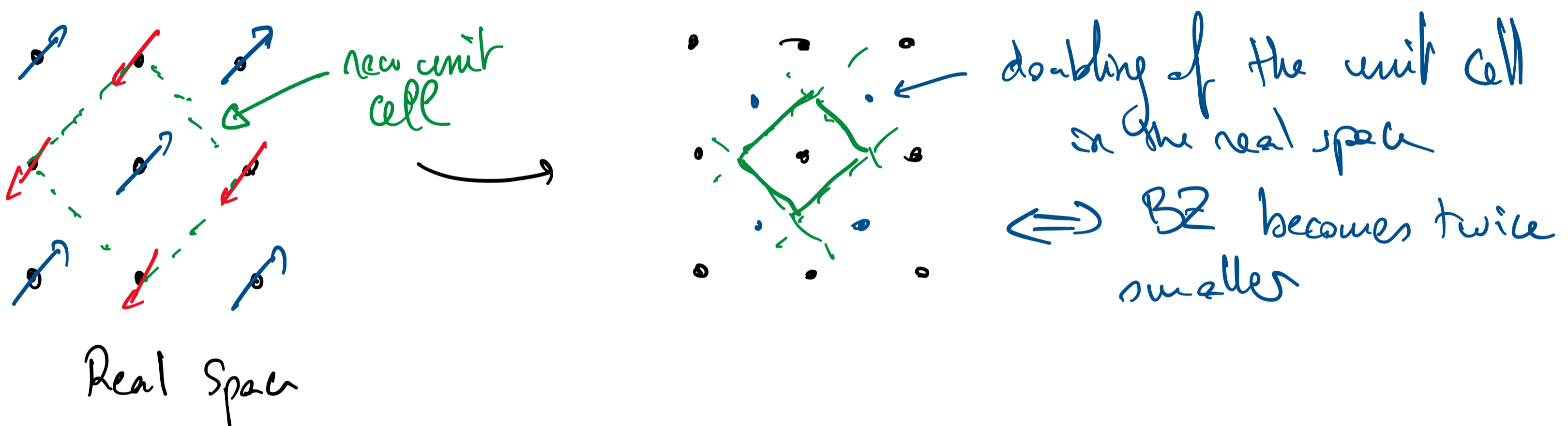


\* Wigner-Seitz cell = Assembly of points which are closer from the origin than from any other point of the lattice



$\Rightarrow$  First Brillouin Zone is the Wigner-Seitz cell of the reciprocal space.

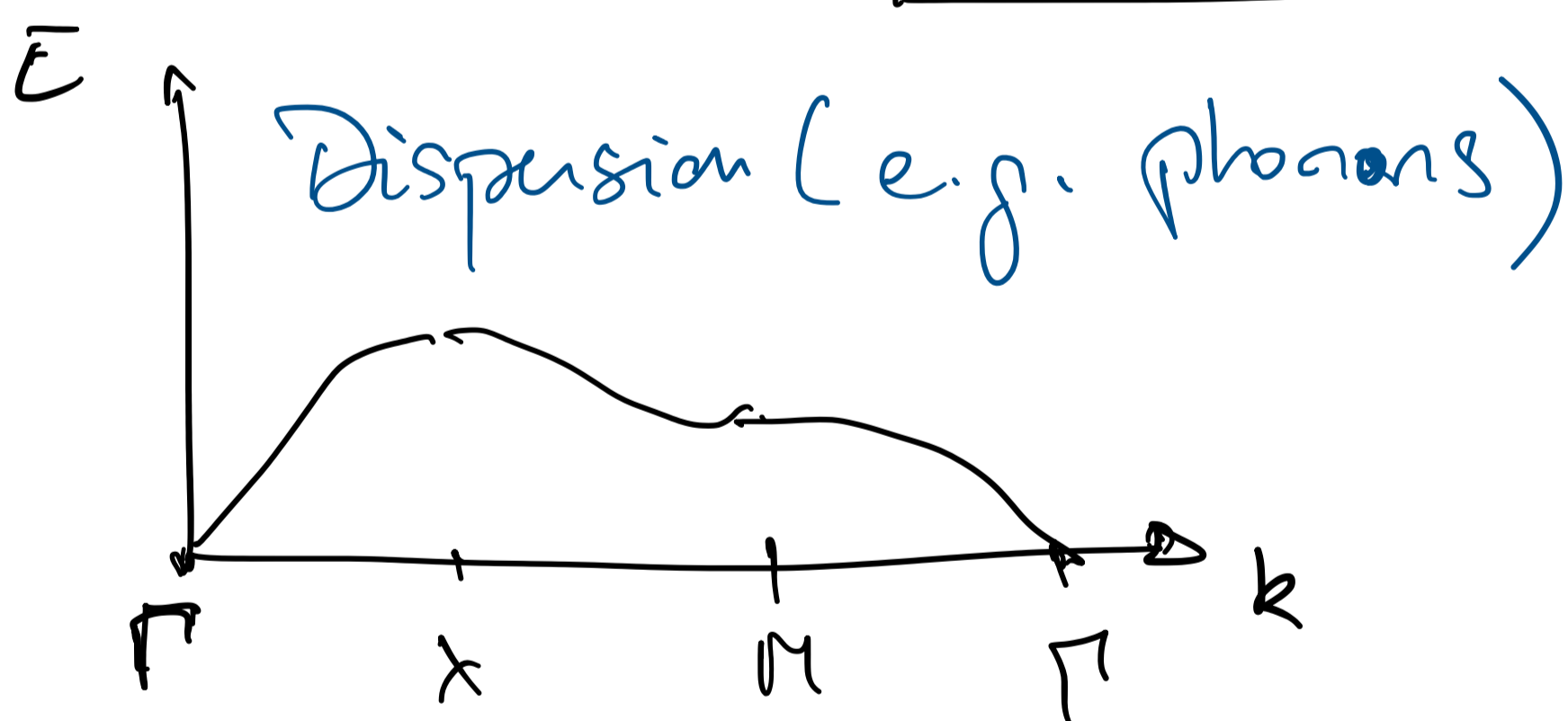
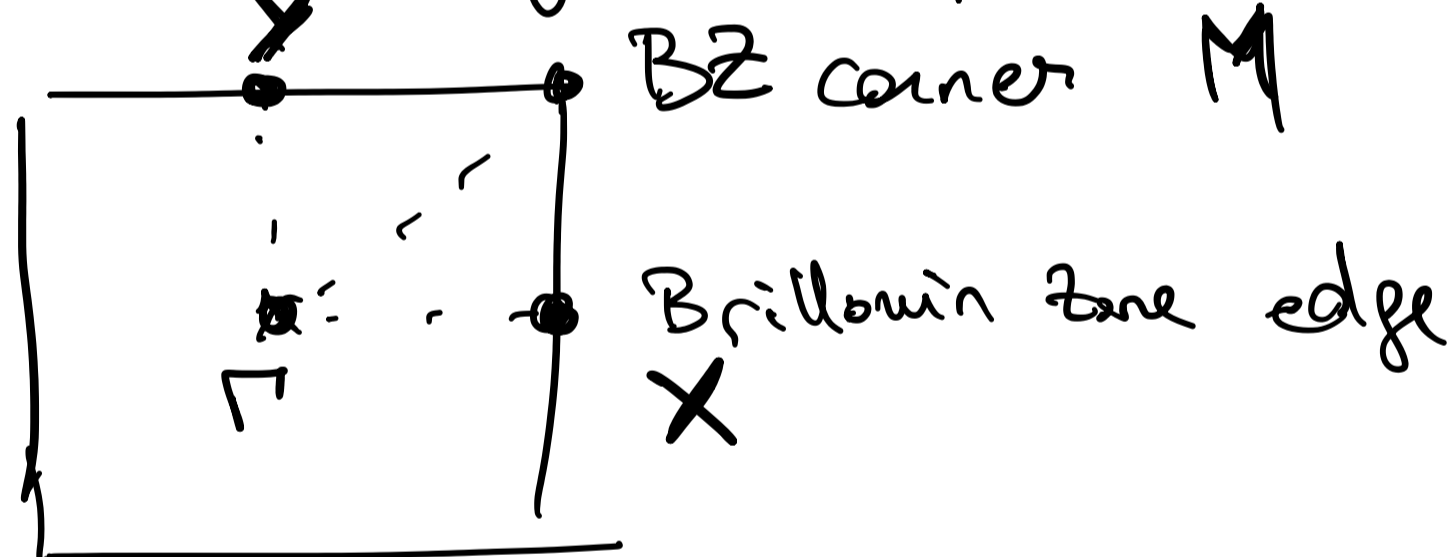
Ex: Doubling of the unit cell in real space (case of Antiferromagnetism)



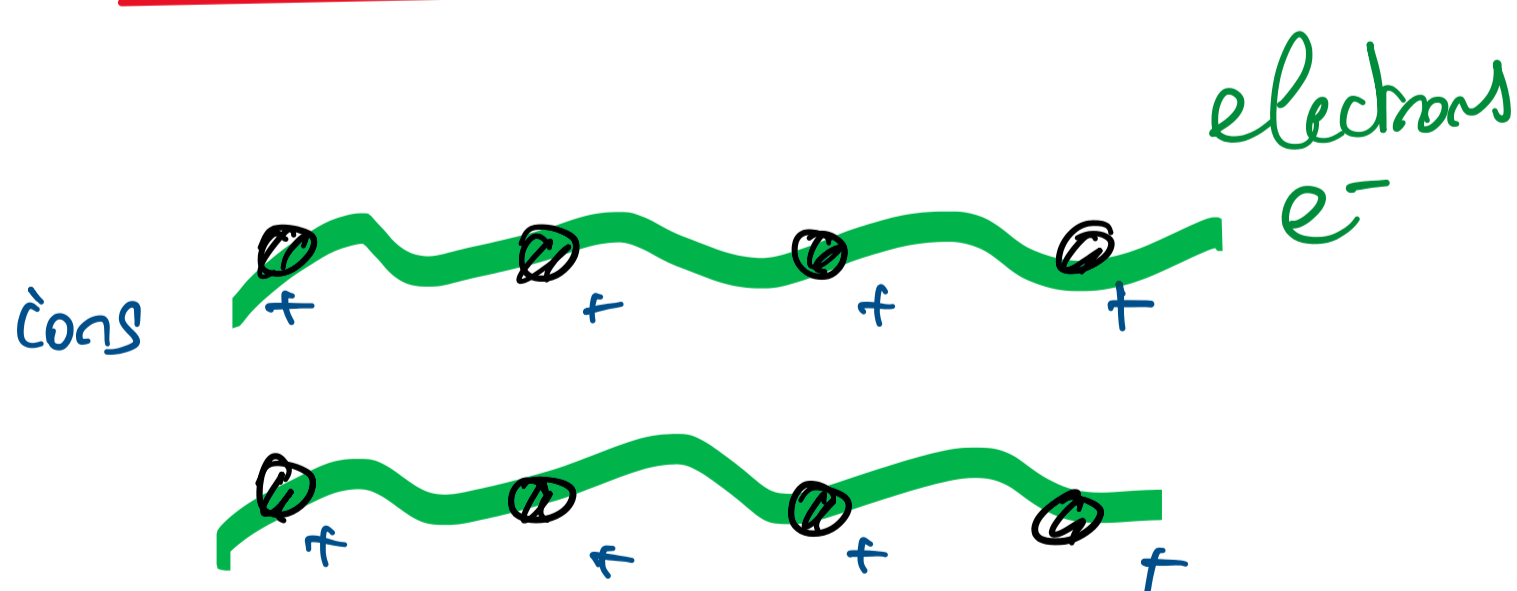
## Special (high symmetry) points

Origin of the reciprocal space

$$\Gamma = \text{gamma point} = (0, 0, 0)$$



## ② Metallic State



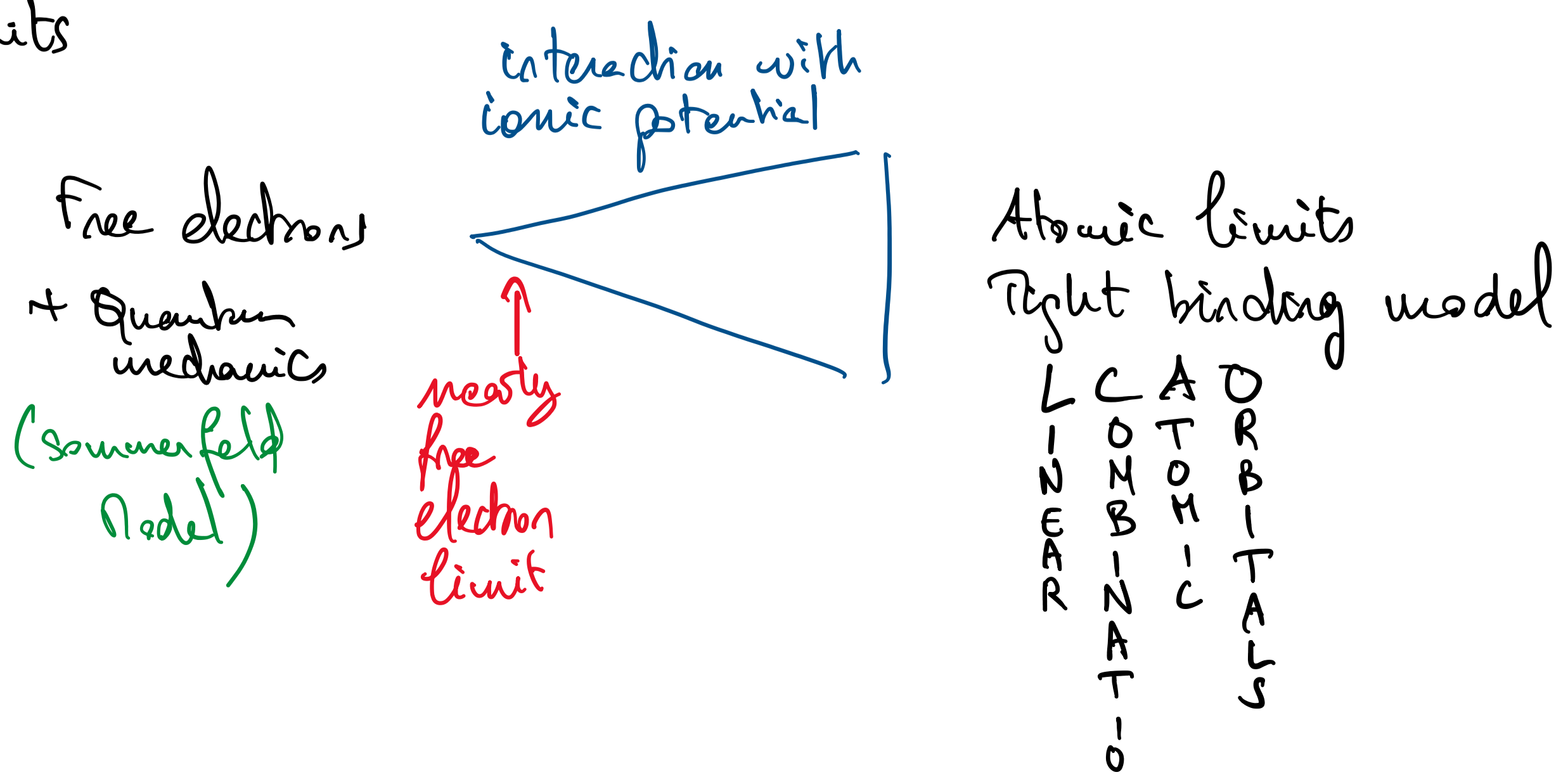
- \* Metallic bonding
- \* Conductions are shared between all the atoms  $\Rightarrow$  delocalized
- \* delocalized act as a "glue" that holds together the ionic lattice.

• Few consequences:

- non-directional bonds = metals are ductile and malleable
- very good electrical and heat conduction
- Efficient screening of electromagnetic waves  $\Rightarrow$  metals are shiny

## ③ Descriptions of electrons in solids

Two limits



Free electrons + Quantum mechanics (Sommerfeld model)

interaction with ionic potential

Atomic limits Tight binding model

LCAO  
NOM  
RBITALS  
NEAR  
NON-  
T  
G