Electrons in a periodic potential

Electrons in a perfectly periodic potential – the Bloch theorem

1D Bravais Lattice

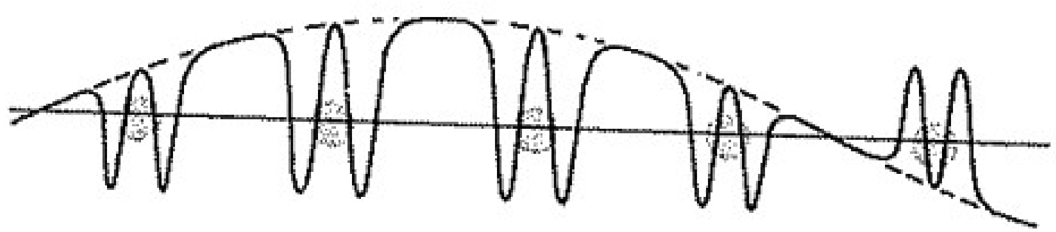
?

$$U(x+a)=U(x)$$

$$\psi(x+a)=\exp(ika)\cdot\psi(x)$$

$$\psi_k(x)=u_k(x)\exp(ikx)$$

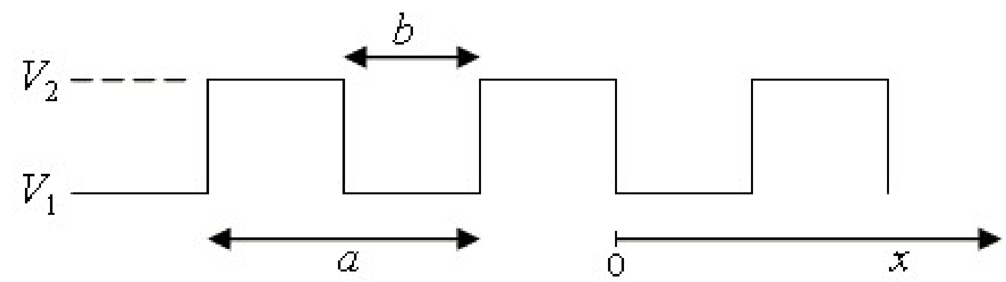
$$u_k(x+a)=u_k(x)$$



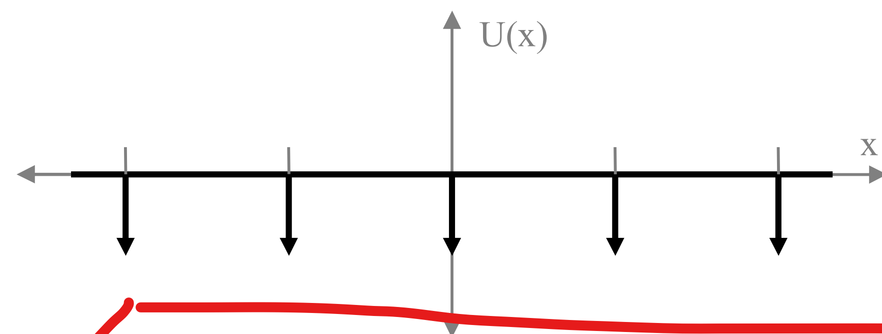
Extended electronic (Bloch) states throughout a periodic solid

Model potentials

Krönig-Penney Model

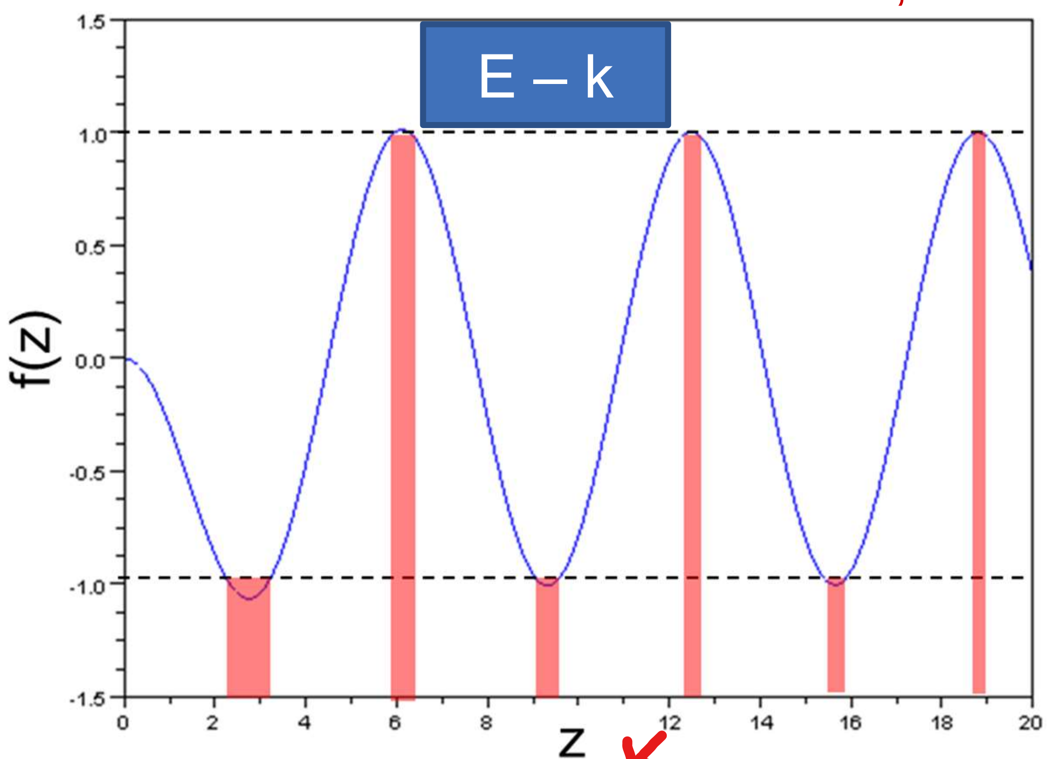


Dirac Comb



?

z, f(z) are the non-linear transformations of k, E



E

k

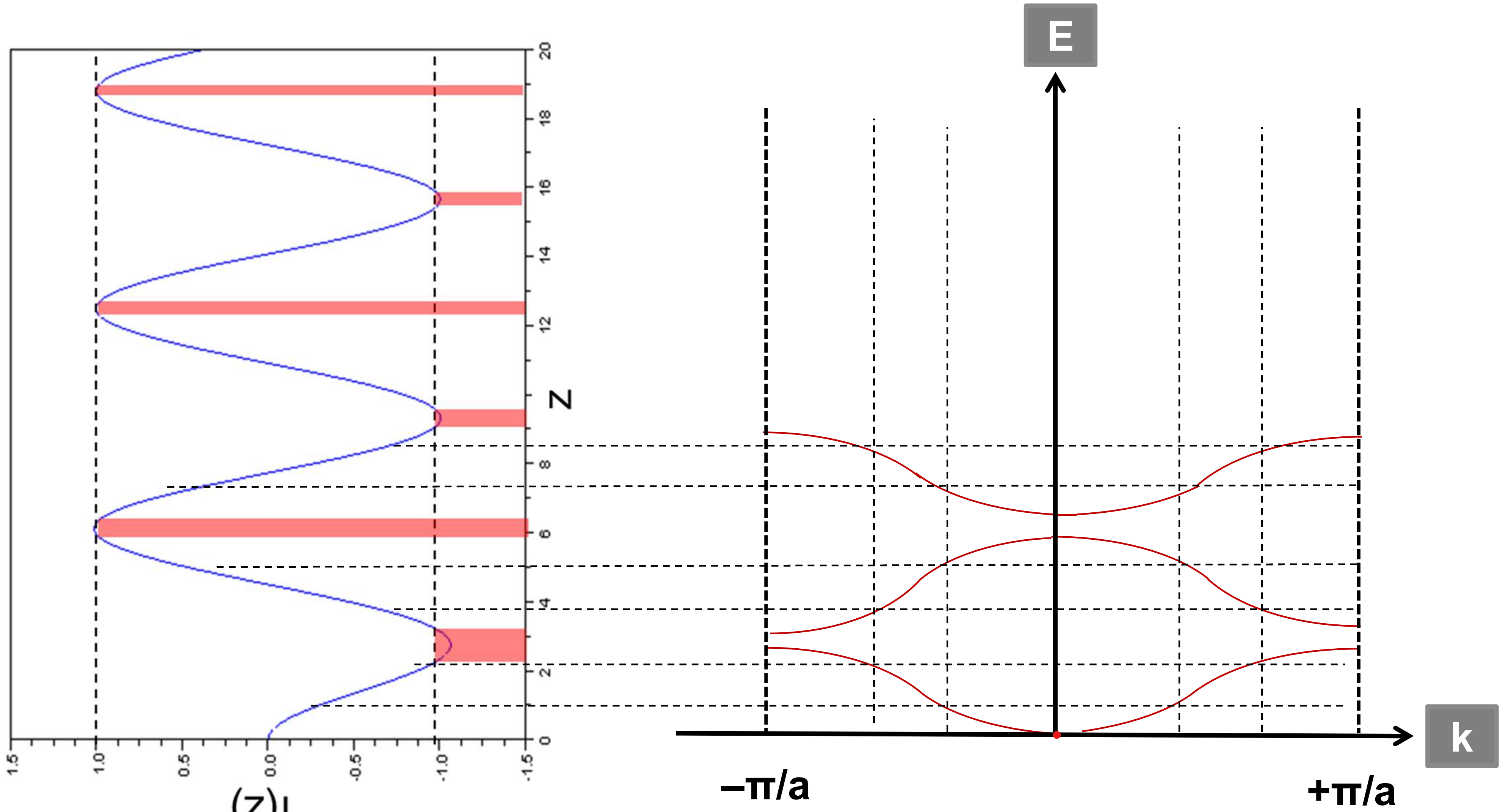
?

$$f(z) = \cos z - \beta \frac{\sin z}{z} = \cos(ka)$$

$$\beta = \frac{m\alpha a}{\hbar^2} \qquad z = qa \qquad q = \sqrt{\frac{2mE}{\hbar^2}}$$

Allowed energy bands and forbidden gaps

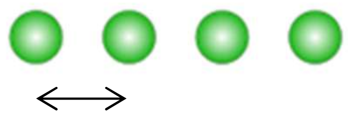
Energy bands (1D)



1st Brillouin Zone (?)

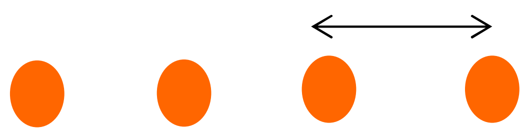
Geometry of (1D) k-space: reciprocal lattice

1D Bravais Lattice
(real space)



a

2π/a



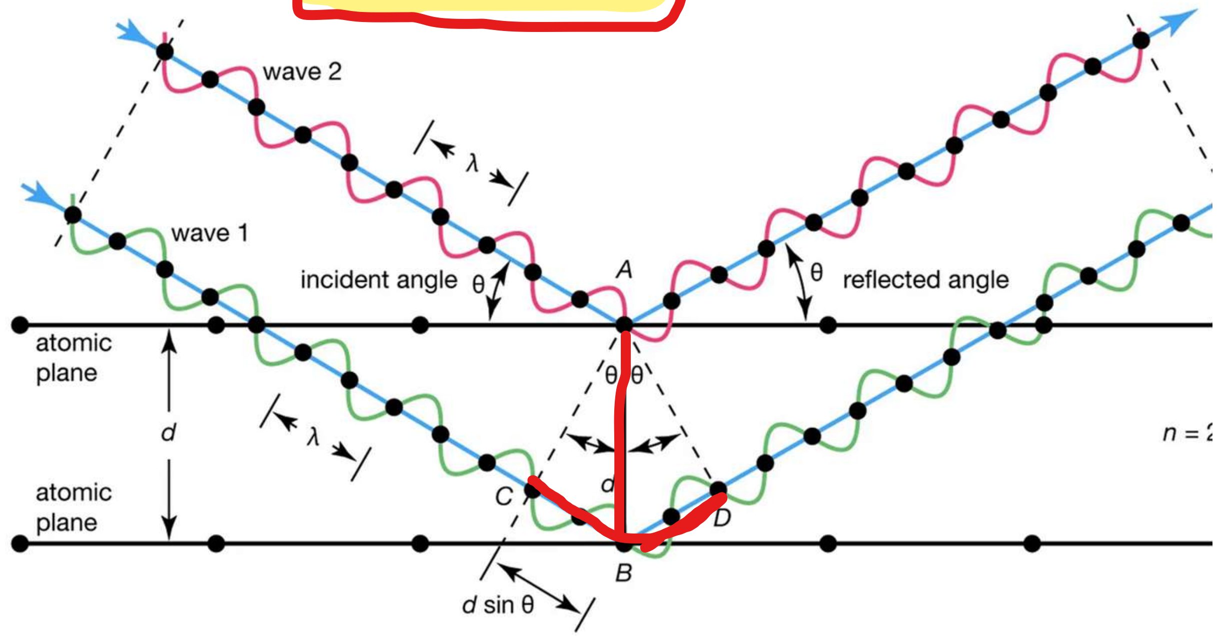
1D B.L. (k-space):
Reciprocal Lattice

1st Brillouin Zone

$$\left[-\frac{\pi}{a}, +\frac{\pi}{a}\right]$$

Bragg Reflection Condition for
wave propagation in crystal

$$2a\sin\theta = n\lambda$$



In 1D

$$2a = n\lambda$$

$$\Rightarrow k = \frac{n\pi}{a}, n \in \mathbb{Z}$$

K vs k ?

Reciprocal Lattice Vector in 1D

$$K = \frac{2n\pi}{a}, n \in \mathbb{Z}$$

Eigenvalues are scalar values that indicate how a square matrix transforms a vector

Energy eigenvalues in (1D) k-space

$$k = k' + K; k' \in 1st\ BZ; K = \frac{2\pi}{a}$$

Mapping higher k to 1st BZ

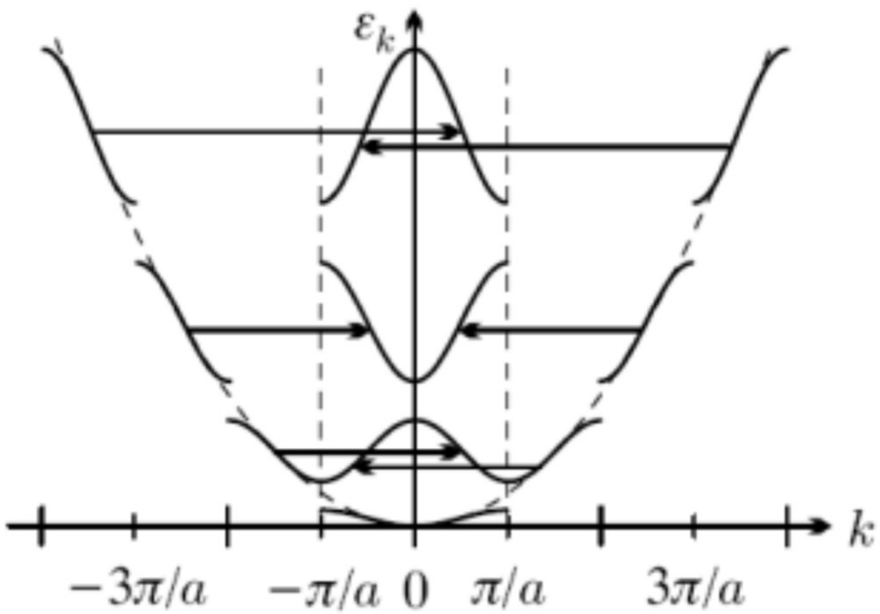
$$\psi_{k'}(x) = e^{ik'x}u_{k'}(x) = e^{i(k-K)x}u_{k'}(x) = e^{ikx}[u_{k'}(x)e^{iKx}] \cong e^{ikx}u_k(x)$$

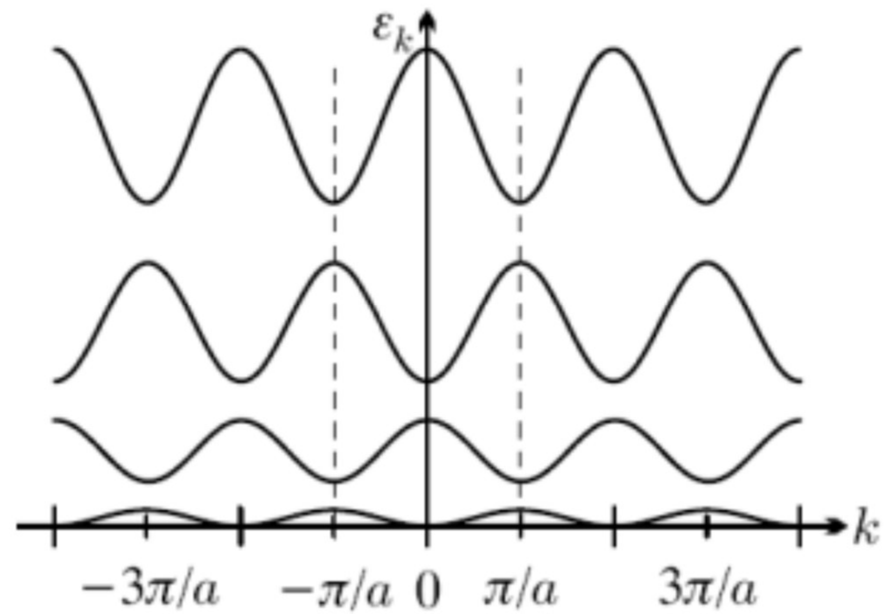
$$|\psi_k|^2 = |\psi_{k'}|^2; |\psi_k|^2 = |\psi_{k'}|^2; E_k = E_{k'}$$

Bandstructure (E-k) is periodic!

Periodic & Extended Zone

Repeated Zone

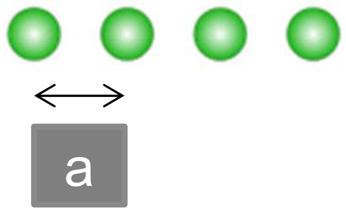




Bandgap opens up at zone boundaries ← Fourier components of periodic potential

Geometry of (1D) k-space: reciprocal lattice

1D Bravais Lattice
(real space)



Periodic Boundary Conditions

→ no boundaries
→ bulk solid

$$\psi(x + Na) = \exp(ikNa) \cdot \psi(x)$$
$$\Rightarrow \exp(ikNa) = 1 = \exp(i2\pi n)$$
$$\Rightarrow k = \frac{2\pi n}{Na}, n \in \mathbb{Z}$$

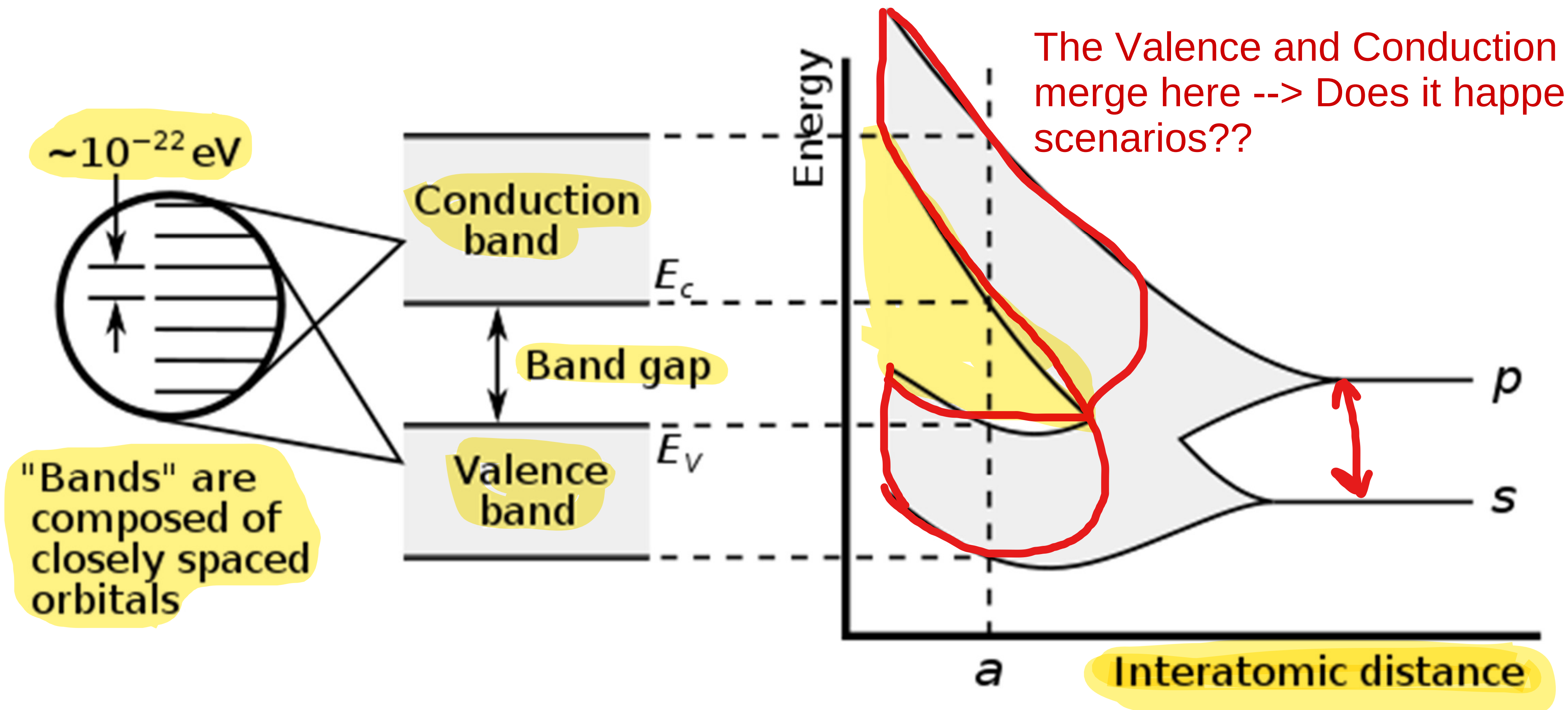
Spacing in reciprocal space

$$\delta k = \frac{2\pi}{Na}$$

No. of k points in 1st BZ = No. of atoms N

	Real-space	k-space
Spacing	a	2π/Na
Range	Na	2π/a

Bands from atomic orbitals



The Valence and Conduction bands merge here --> Does it happen in all the scenarios??

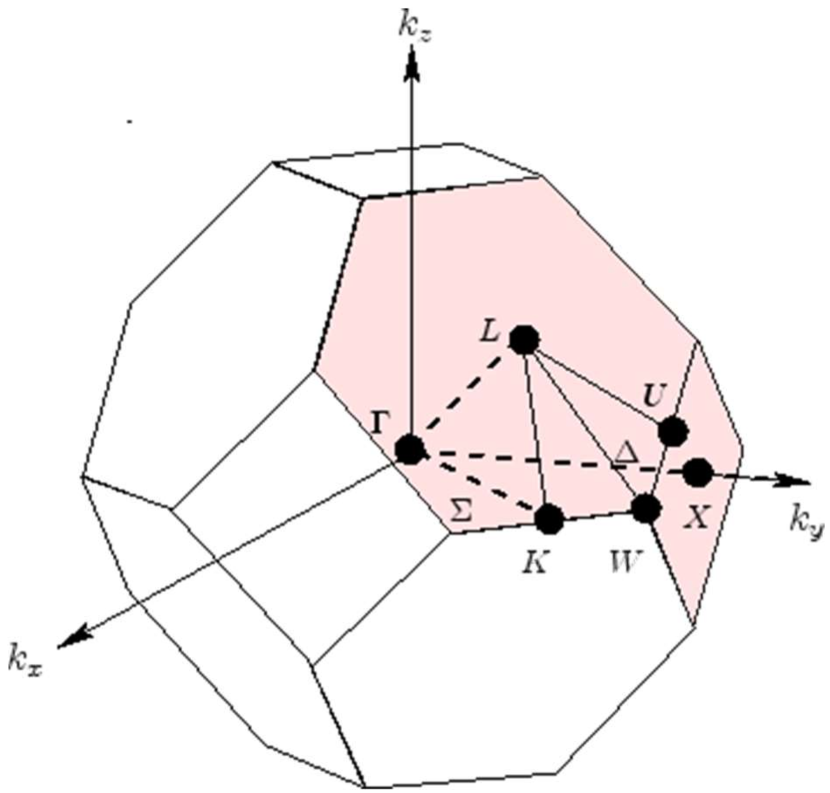
Reciprocal lattice in 2D, 3D

K. R = 0 The Vectors are perpendicular to each other.

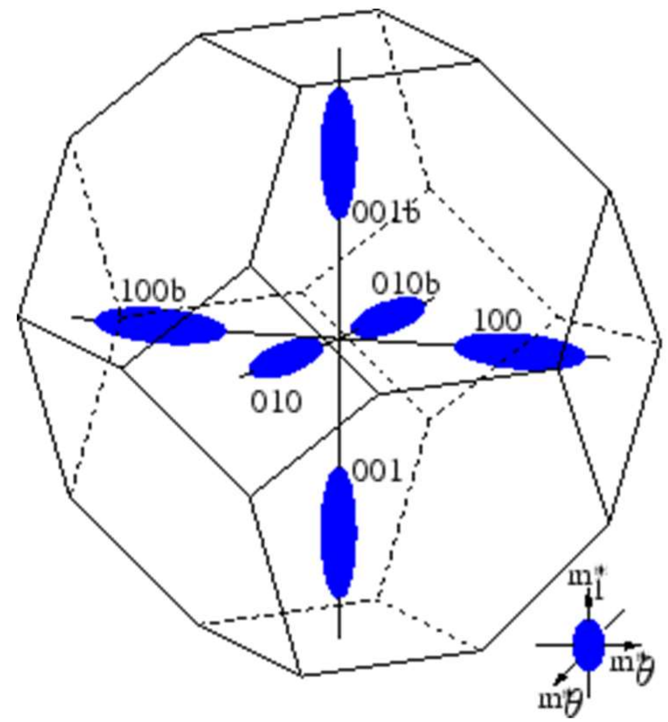
Set of points in k-space

$$\boxed{\left\{\vec{K}\right\}:\exp\left(i\vec{K}\cdot\vec{R}\right)=1}$$

Verify for 1D



1st BZ of FCC



Si CB minima

What is reciprocal of reciprocal lattice?

The normal lattice.

Finis

Artwork Sources:

1. en.wikipedia.org
2. iue.tuwien.ac.at
3. www.wikipedia.com
4. www.Britannica.com
5. Kalt & Klingshirn, Springer
6. Souvik Mahapatra (IITB)
7. https://physics.iisc.ac.in/~aveek_bid/wp-content/uploads/2019/07/