Brillouin Zones (reciprocal space):

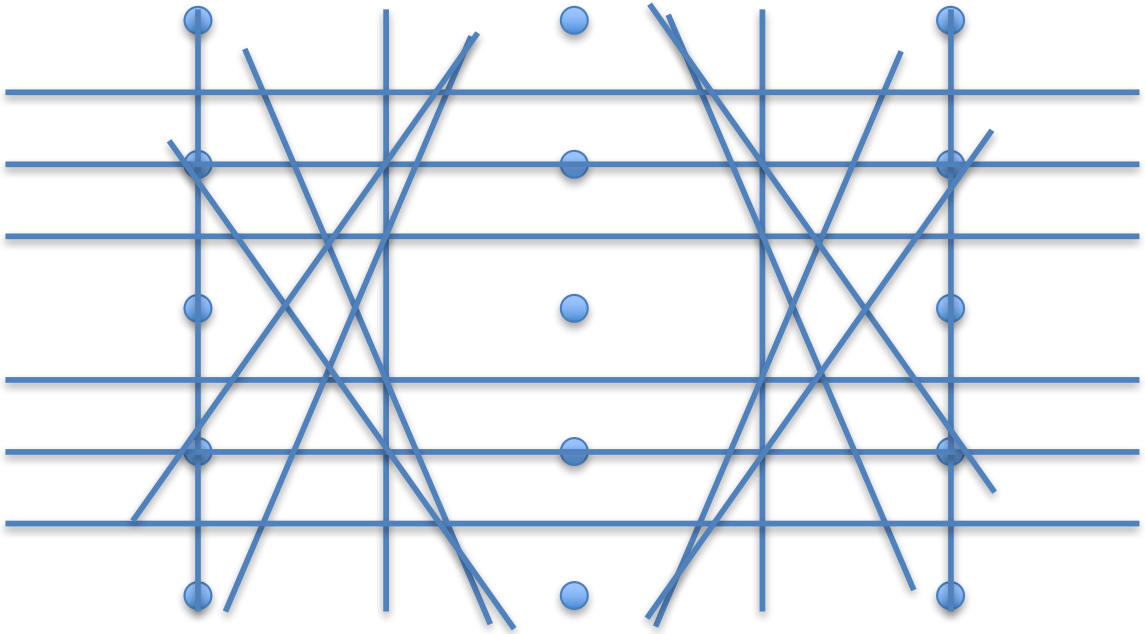
Mth zone: Spatial region(s) having **origin as Mth nearest *K* point**. Equivalent: Space reached from origin by **crossing (M - 1) perpendicular bisector planes**.

- Each zone contains *N k* points (e.g. *k* defined with periodic boundary conditions, *N* = number of Bravais-lattice cells in crystal).

$$\vec{b}_1 \cdot \vec{b}_2 \times \vec{b}_3 = (2\pi)^3 / \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3$$

- All zones same volume; can "fold into 1st zone" by translation through *K*.
- Result: each zone holds 2 electrons per Bravais-lattice cell.

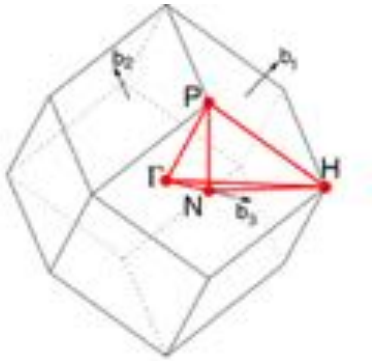
2D example

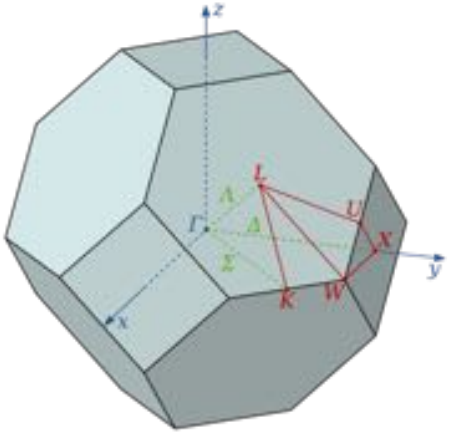


3D Brillouin Zones:

FCC 1st Brillouin zone (image: Wikipedia). • Brillouin zones relate only to Bravais lattice; applies to FCC elements (Cu, Al…) or with basis (silicon, GaAs, etc.).

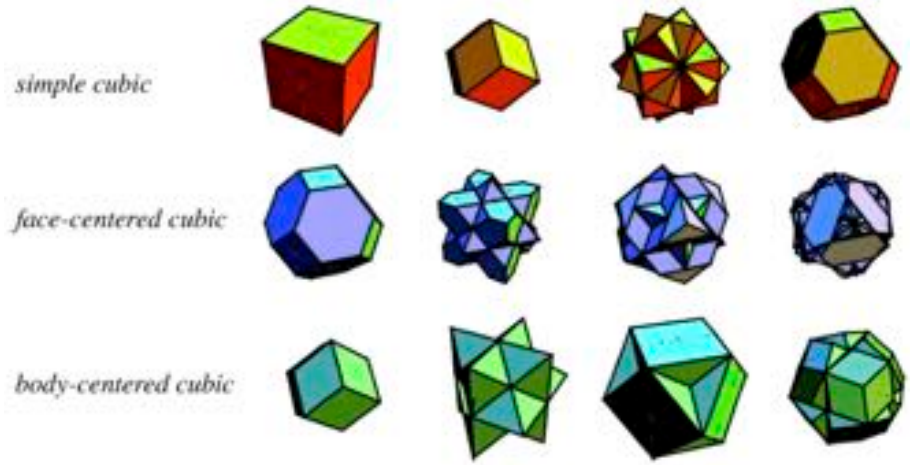
BCC 1st Brillouin zone.



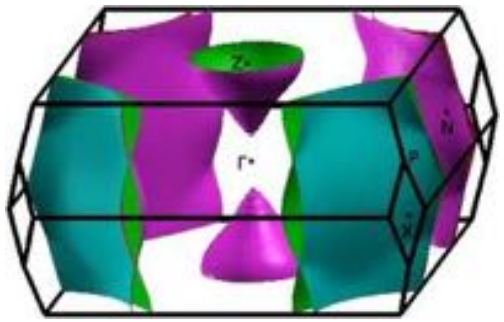


Labels: center ($k = 0$) always Γ, other labels by historical convention (L, X, etc.)

Cubic structures , first 4 zones in extended space: (image from MathWorld)

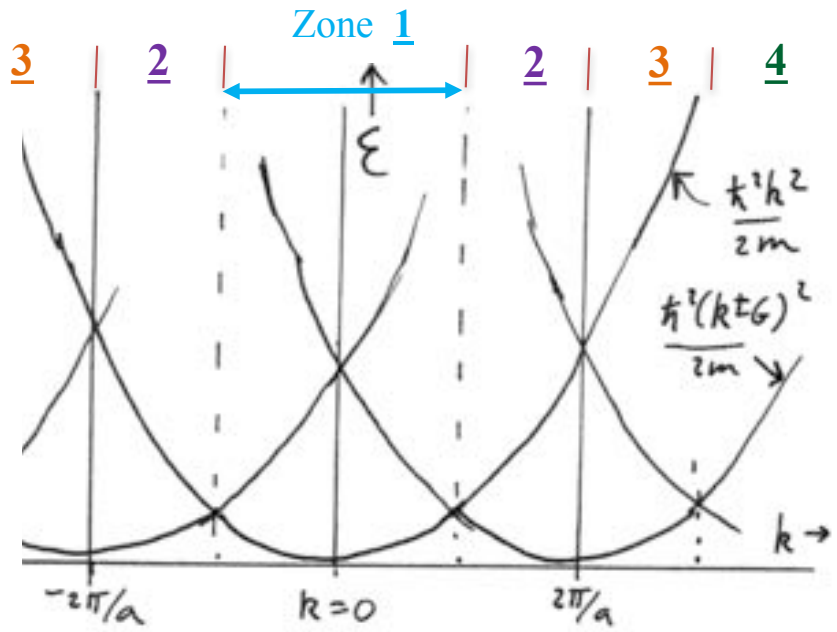


Body centered tetragonal, 1st zone with KFe_2Se_2 superconductor Fermi surface (Liu et al. Physica B 407, 1139, 2012)

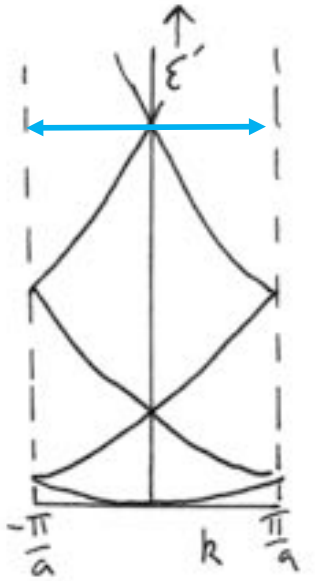


"Nearly-free electron model": weak periodic potential.

Free-electron states, Extended zone scheme



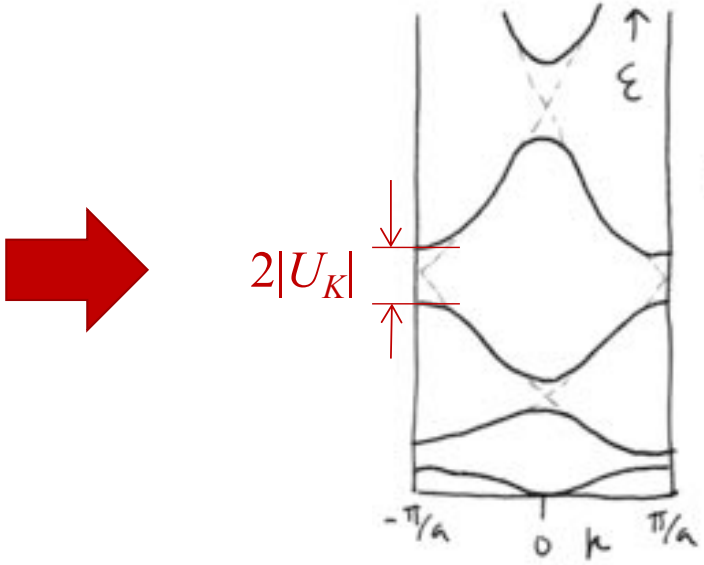
folded into 1BZ =
reduced zone scheme.



1-d bands "Folded"

(free electrons)

One BZ contains set of distinct eigenfunctions



1-d with perturbation = periodic potential.

Nearly-Free electron model:

$$U(\vec{r}) = \sum_K U_{\vec{K}} e^{i\vec{K}\cdot\vec{r}} \qquad \psi_i = u(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = \left(\sum_K \alpha_{k,K} e^{i\vec{K}\cdot\vec{r}} \right) e^{i\vec{k}\cdot\vec{r}}$$

Bloch states

Assume *U* weak; perturbation theory $\varepsilon_o(k) \equiv \dfrac{\hbar^2 k^2}{2m}$

through 2nd order:

$$\varepsilon = \frac{\hbar^2 k^2}{2m} + \sum_K \frac{|U_K|^2}{\varepsilon_o(\vec{k}) - \varepsilon_o(\vec{k} - \vec{K})}$$

- As before, U joins only states $k \pm K$.
- Small energy changes except when states are degenerate.
- Degeneracies: always on Brillouin Zone Boundaries.