* Single-electron states in a periodic potential

→ Bloch wavefunctions that share the periodicity of the lattice

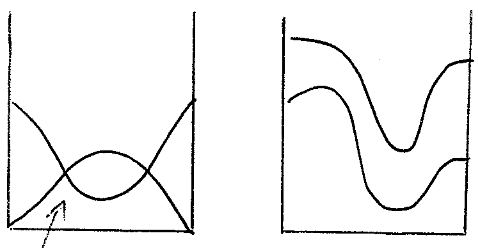
→ characterized by quantum numbers k, n, σ ← spin projection

wavevector in the BZ

band index

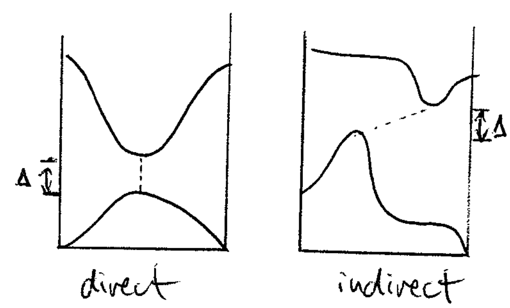
→ dispersion relation $\varepsilon_{\vec{k},n} = \varepsilon_n(\vec{k})$ maps out a discrete (in n) set of continuous (in k) bands

→ various possibilities for the "spaghetti" of bands



band crossing protected by symmetry

ungapped



gapped

→ bands filled according to the Fermi-Dirac distribution

$$\frac{1}{e^{(\varepsilon_{\vec{k},n} - \mu)/k_B T} + 1}$$

for a system in thermal equilibrium at temp T

* Fermi surface is defined in the low-temperature limit as the demarkation between filled and unfilled states

→ states filled below the fermi energy $\mu \to \varepsilon_F$ as $T \to 0$

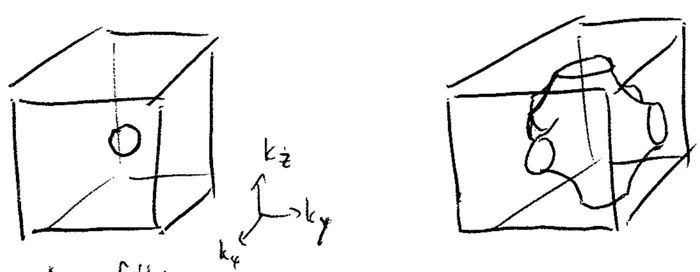
→ $$\langle c^\dagger_{k,n} c_{k,n} \rangle = \begin{cases} 1 & \varepsilon_{k,n} < \varepsilon_F \\ 0 & \varepsilon_{k,n} > \varepsilon_F \end{cases}$$

→ for free electrons $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$, all level surfaces of the dispersion are spherical; $\varepsilon_k = \varepsilon_F$ picks out all points at radius $k_F = \frac{\sqrt{2m\varepsilon_F}}{\hbar}$ in k-space

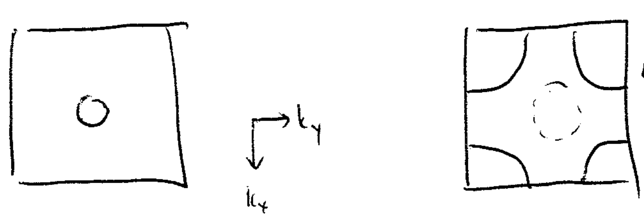
→ generic fermi surfaces deviate from spherical shape, especially near BZ boundaries

e.g. cubic tight-binding band...

$$\varepsilon_k = -2t\,(\cos k_x a + \cos k_y a + \cos k_z a)$$



low filling

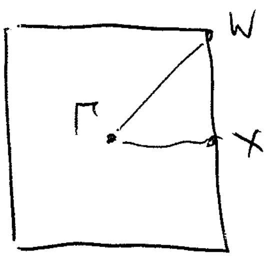


bands intersect normal to the zone edge

* Non-spherical Fermi surfaces open up two important new possibilities

① large density of states at the Fermi level

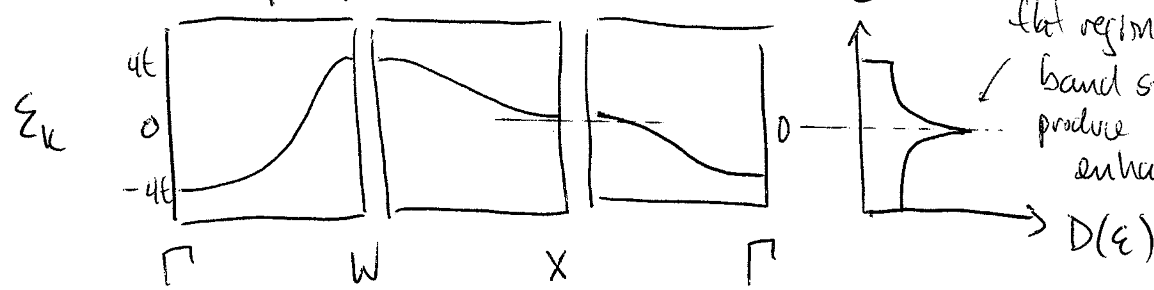
e.g. square tight-binding band $\varepsilon_k = -2t(\cos k_x a + \cos k_y a)$



standard labelling of high-symmetry points in the BZ

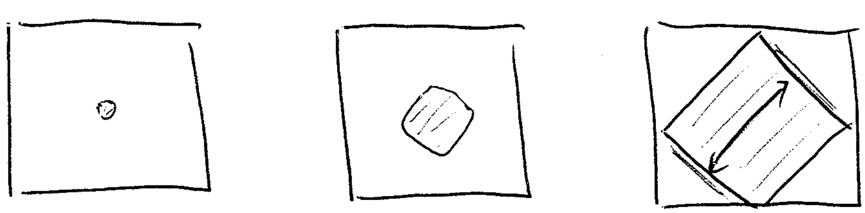
BZ

plot paths through BZ



flat regions of band structure produce large DOS enhancements

② a single wavevector $\vec{Q}$ may connect nontrivial subsets of the FS



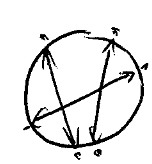
low filling

quarter filling

half filling

nesting vector $\vec{Q} = (\pi, \pi)$

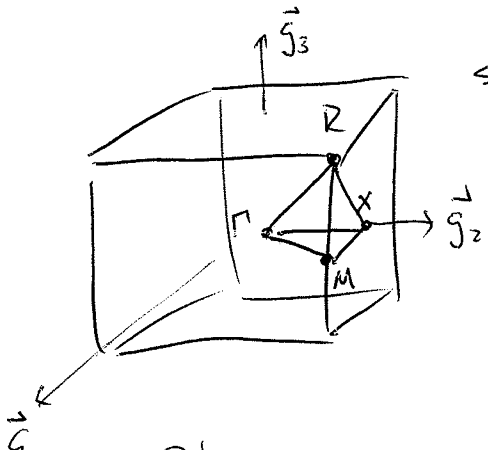
cf sphere: each vector connects only two points



→ large DOS at the Fermi level and the existence of a nesting vector tend to drive instabilities to unusual forms of order (magnetism, superconductivity, lattice distortions)

Cubic lattice system

simple cubic

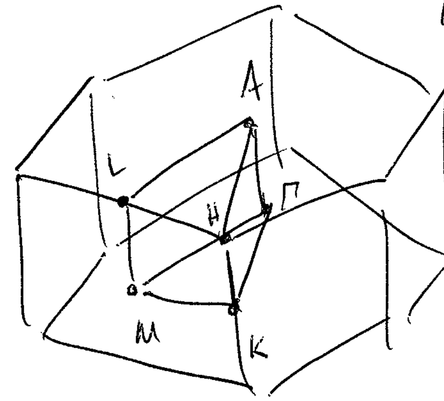


e.g. Paths

Γ–X–M–Γ–R–X

M–R

hexagonal

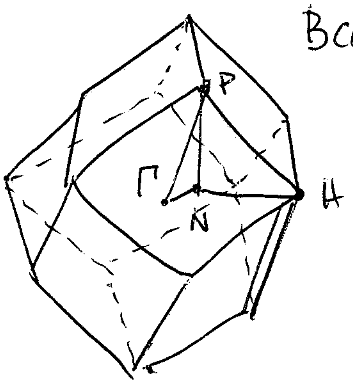


Γ–M–K–Γ–A–L–H–A

L–M

K–H

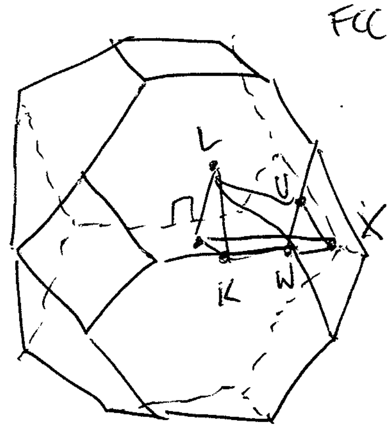
BCC



Γ–H–N–Γ–P–H

P–N

FCC

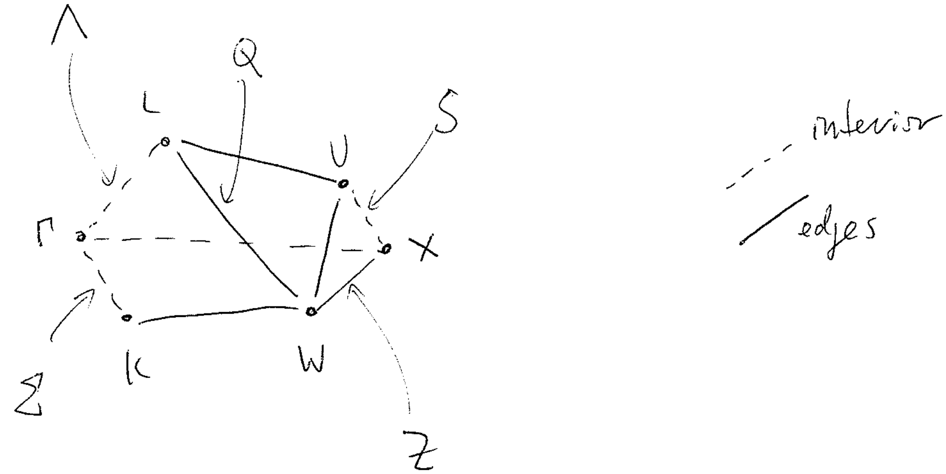


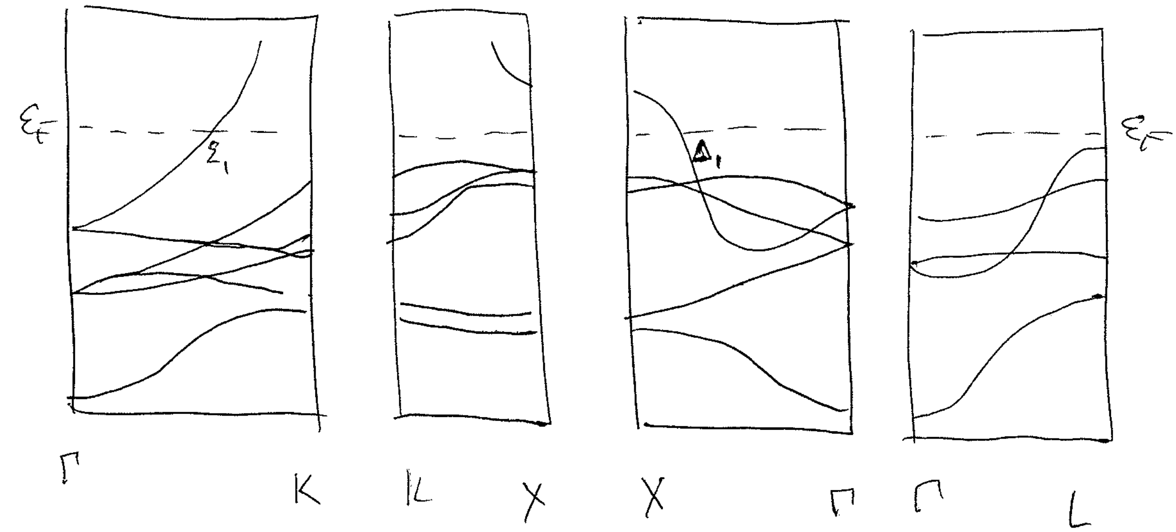
Γ–X–W–K–Γ–L–U–W–L–K

U–X

* Sometimes use additional path labels

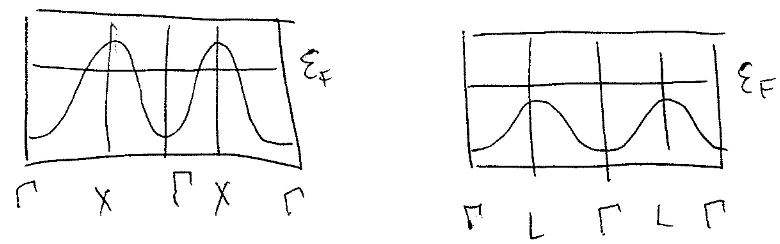
FCC





Copper has Σ_1 and Δ_1 bands crossing the fermi surface.

NB



gapped

* Response to forces

→ apply $\vec{F}_{ext} = \quad -e\,[\vec{E} + \vec{v}\times\vec{B}]$

→ $m\langle\dot{\vec{v}}\rangle = \vec{F}_{ext} + \langle\vec{F}_{lattice}\rangle$

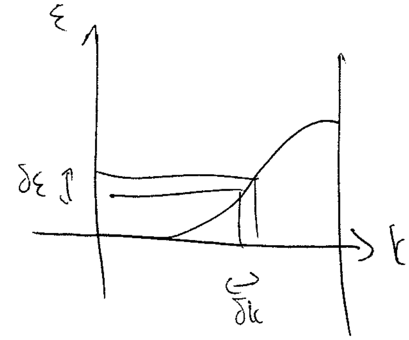
↑ scattering and relaxation processes

→ e.g. 1D

$$\delta\varepsilon = F_{ext}\, v\, dt = \left(\frac{\partial\varepsilon}{\partial k}\right)\delta k = \hbar v\,\delta k$$

$$\Rightarrow F_{ext}\,\delta t = \hbar\,\delta k$$

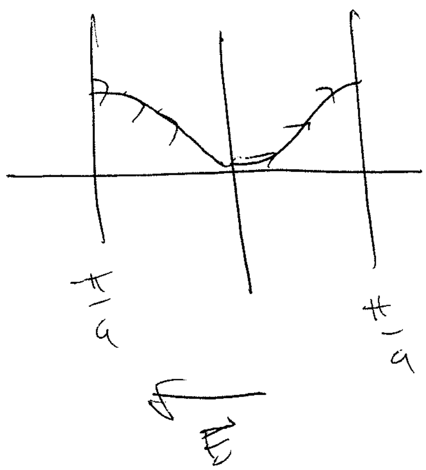
$$\Rightarrow F_{ext} = \hbar\dot{k}$$



(argument cannot apply to $\vec{v}\times\vec{B}$ term since force ⊥ velocity imparts no energy)

Even though argument fails,

$$F_{ext} = \hbar\dot{\vec{k}} = -e\,(\vec{E} + \vec{v}\times\vec{B})$$



* Constant electric field

→ Bragg reflection since w.f. on the Bragg planes are identical

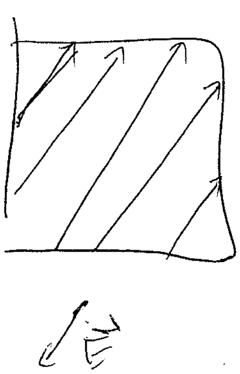
→ gradient goes +ve and −ve, so that electron oscillates back and forth (Bloch oscillations)

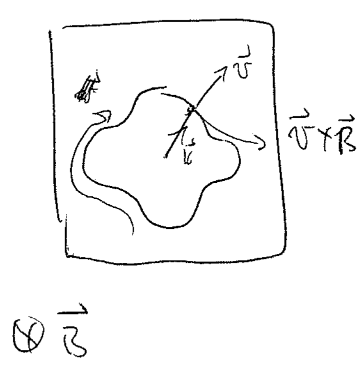
→ i.e. DC electric field ⇒ oscillating current (~100 GHz)

we don't see this

→ electron is scattered so often that it never completes a cycle

→ can be done with $\vec{B}$ field

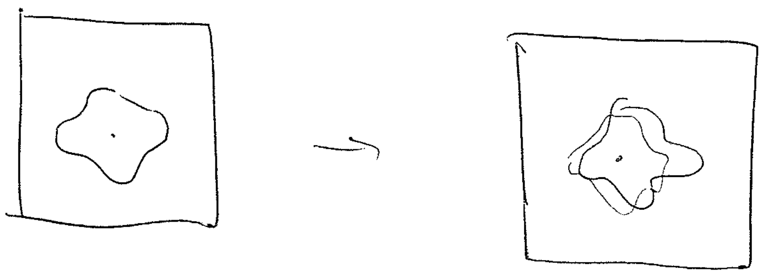




$$\vec{v} \times \vec{B}\, \delta t = \hbar \delta k$$

for free electrons

⇒ cyclotron frequency with $\omega = \frac{eB}{m}$



$\underline{E} = 0$ $\qquad\qquad$ $\underline{E}$

$$j = \quad \sim \sum_n \int \frac{d^3k}{(2\pi)^3} \frac{\vec{\nabla} \varepsilon_{k,n}}{e^{\beta(\varepsilon_{k,n}-\mu)}+1}$$

→ time reversal symmetry $\varepsilon_\uparrow(k) = \varepsilon_\downarrow(-k) \Rightarrow \varepsilon_k = \varepsilon_{-k}$

$$v_{-k} = -v_k$$

→ filled bands inert: $\underset{\substack{\uparrow \\ \text{filled} \\ \text{band } n}}{j_n} = \int \frac{d^3k}{(2\pi)^3} \nabla \varepsilon_{k,n} \equiv 0$