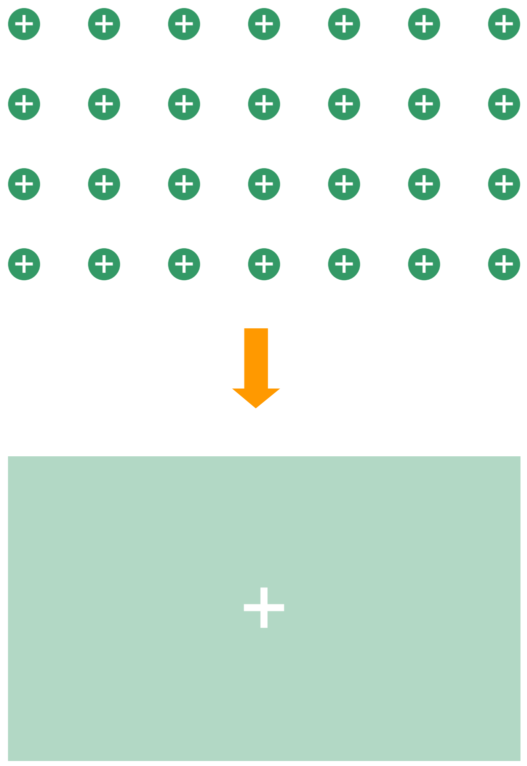
simple metals - Jellium model

smearing of the ion-lattice

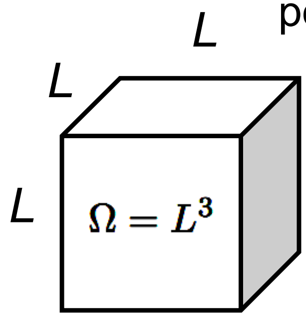


$n_{ion} = n_e$

charge neutrality

free electron states

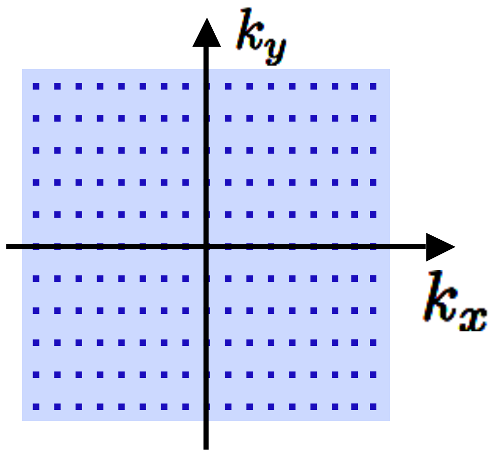
$$\psi_{\vec{k},s}(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}}$$



periodic boundary conditions

$$\psi_{\vec{k},s}(\vec{r} + L\hat{x}) = \psi_{\vec{k},s}(\vec{r} + L\hat{y})$$

$$= \psi_{\vec{k},s}(\vec{r} + L\hat{z}) = \psi_{\vec{k},s}(\vec{r})$$



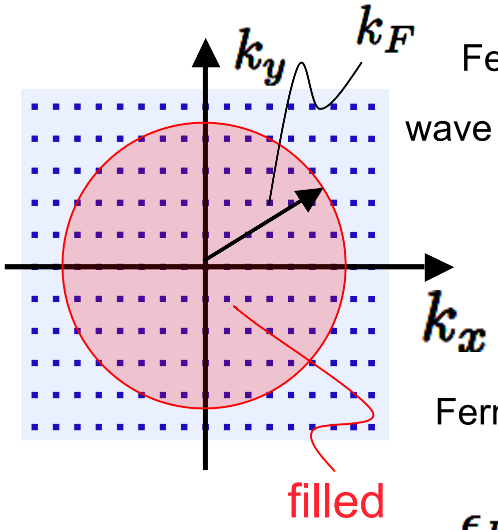
wave vector

$$\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$$

energy

$$\epsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$$

simple metals - Jellium model



Fermi energy

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

ground state: *N* electrons

$$|\Psi_0\rangle = \prod_{|\vec{k}|\le k_F} \prod_s \hat{c}^\dagger_{\vec{k},s}|0\rangle \qquad \epsilon_{\vec{k}} \le \epsilon_F$$

$$N = \sum_{|\vec{k}|\le k_F, s} 1$$

$$= 2\Omega \int \frac{d^3k}{(2\pi)^3}\Theta(\epsilon_F - \epsilon_{\vec{k}}) = 2\frac{4\pi}{3}\frac{\Omega k_F^3}{(2\pi)^3}$$

Fermi wave vector
versus electron density

$$k_F = (3\pi^2 n)^{1/3}$$

$$n = \left(\frac{4\pi}{3}d^3\right)^{-1} \Rightarrow k_F = \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{d}$$

radius of volume per mobile electron

$$d \sim 2\text{Å} \Rightarrow k_F \sim 10^8\,\text{cm}^{-1}$$

simple metals - Fermi surfaces

ideal elemental metals:

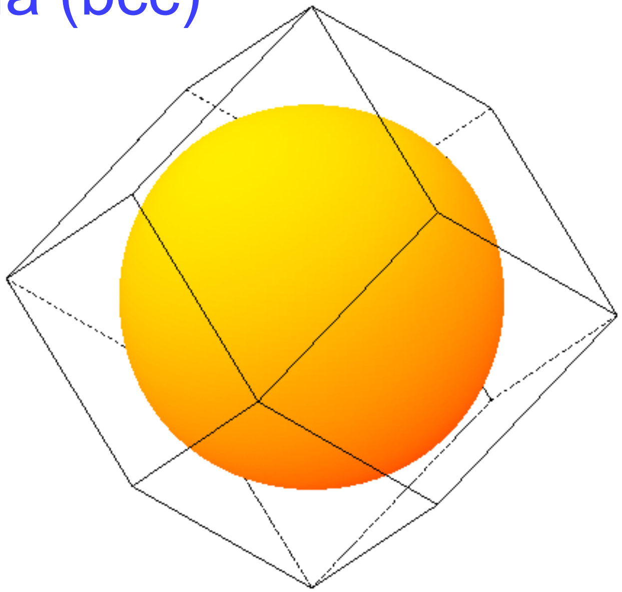
alkali metals (group I)

Li, Na, K, Rb, Cs

[noble gas] $(ns)^1$

half-filled band

Na (bcc)

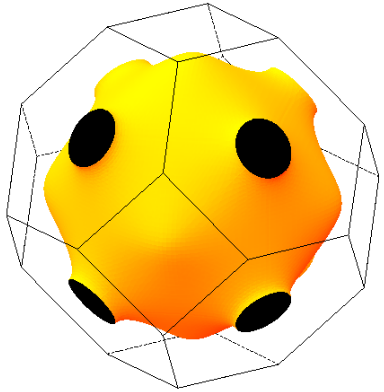


like parabolic band

nobel metals

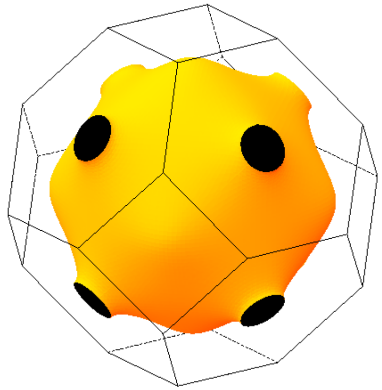
Cu (fcc)

$[Ar](3d)^{10}(4s)^1$



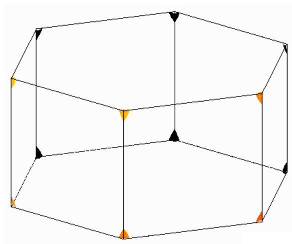
Ag (fcc)

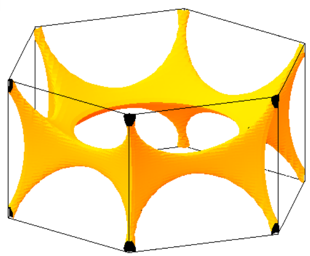
$[Kr](4d)^{10}(5s)^1$

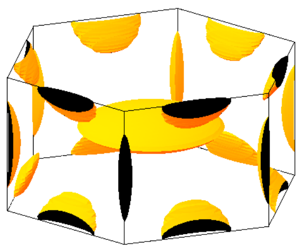


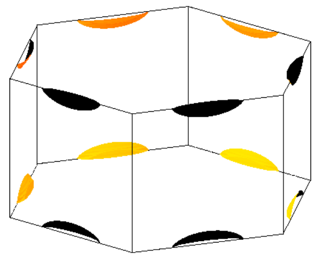
non-ideal metal: Mg (hcp)

$[Ne](3s)^2$









overlapping bands

Fermi surface explorer:

http://www.phy.tu-dresden.de/~fermisur/