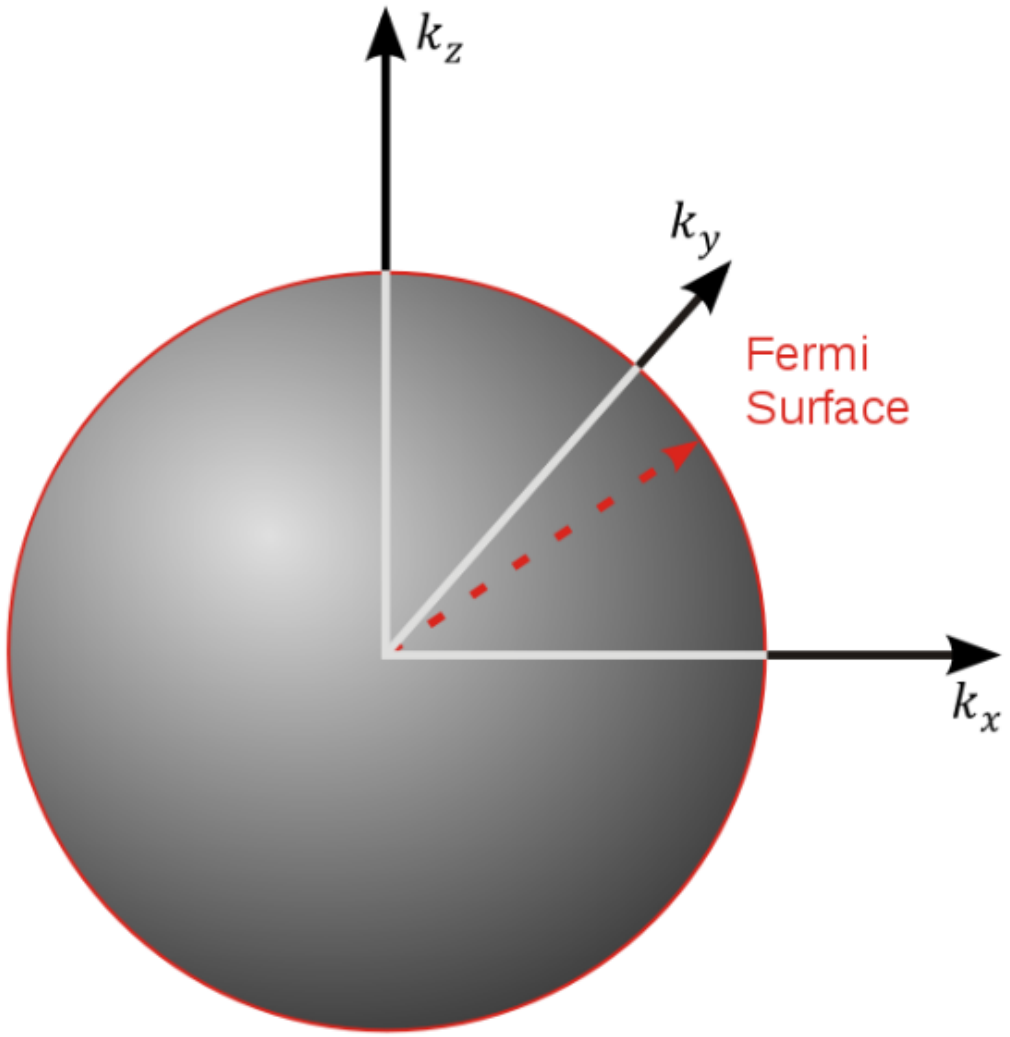
3. Metals

Oct 10, 2019

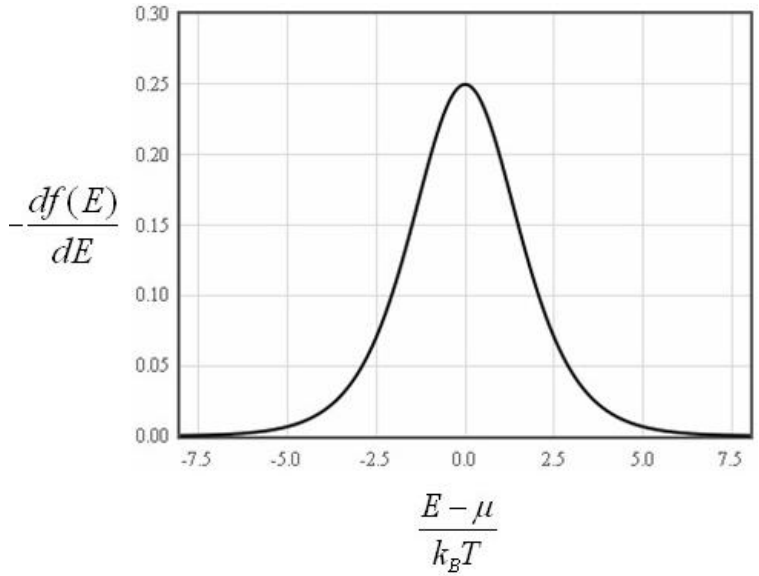
Fermi surface for free electrons



Properties of metals depend mostly on the electron states at the Fermi surface

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE = \int_{-\infty}^{\infty} \frac{D(E) dE}{\exp\left(\frac{E-\mu}{k_B T}\right)+1}.$$

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE = K(\infty) f(\infty) - K(-\infty) f(-\infty) - \int_{-\infty}^{\infty} K(E) \frac{f(E)}{dE} dE.$$



http://lampx.tugraz.at/~hadley/ss1/materials/thermo/dos2mu.html

Thermodynamic properties

Chemical potential (implicitly defined by):

$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1+\exp\left(\frac{(E-\mu)}{k_B T}\right)} dE$$

DoS → mu

Internal energy density:

$$u = \phi + Ts + \mu n = \int_{-\infty}^{\infty} \frac{ED(E)}{1+\exp\left(\frac{E-\mu}{k_B T}\right)} dE$$

DoS → u(T)

Energy spectral density:

$$u(E,T) = \frac{ED(E)}{1+\exp\left(\frac{E-\mu}{k_B T}\right)}$$

DoS → u(E)

Specific heat:

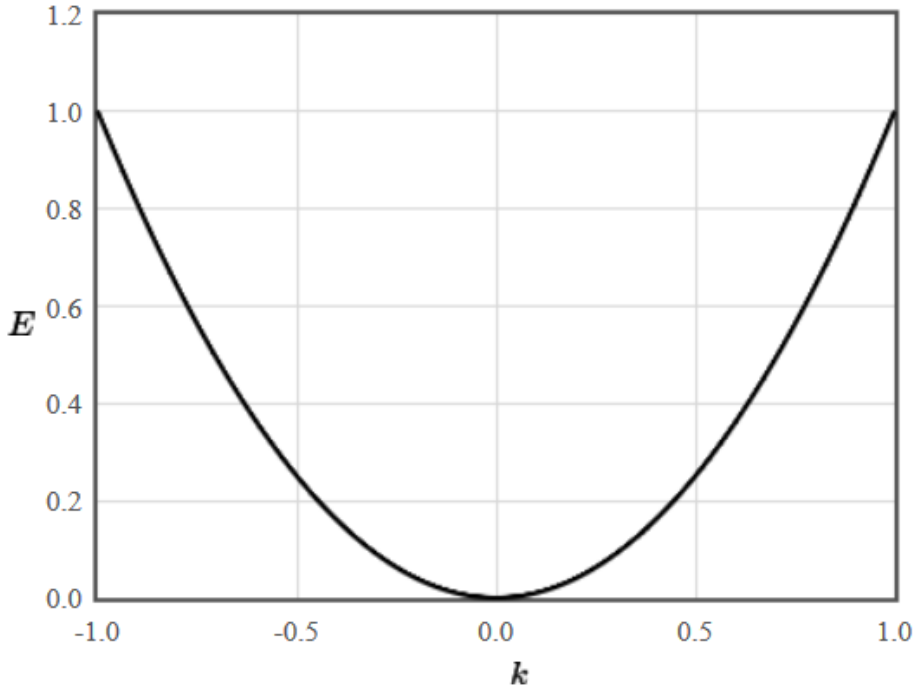
$$c_v = \frac{\partial u}{\partial T} = \int_{-\infty}^{\infty} \frac{ED(E)(E-\mu)\exp\left(\frac{E-\mu}{k_B T}\right)}{k_B T^2 \left(1+\exp\left(\frac{E-\mu}{k_B T}\right)\right)^2} dE$$

DoS → cv(T)

http://lamp.tu-graz.ac.at/~hadley/ss2/fermigas/thermo/thermo.php

Empty lattice approximation

Free electrons cannot absorb photons



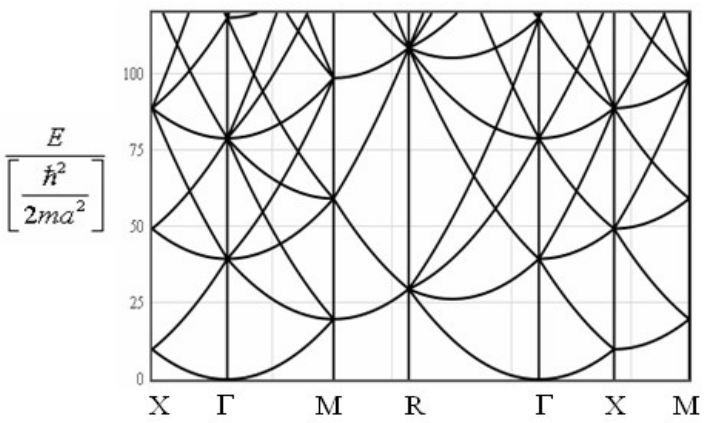
$$\hbar\vec{k}_f = \hbar\vec{k}_i + \hbar\vec{G}$$

$$\vec{k}_f - \vec{k}_i = \vec{G}$$

Laue condition

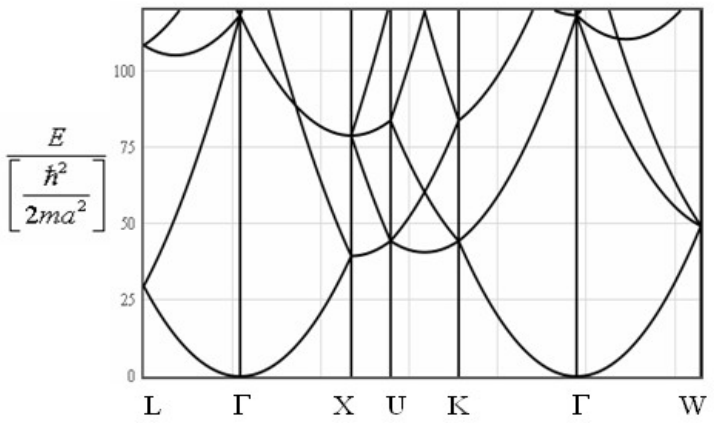
Empty lattice approximation

Simple cubic



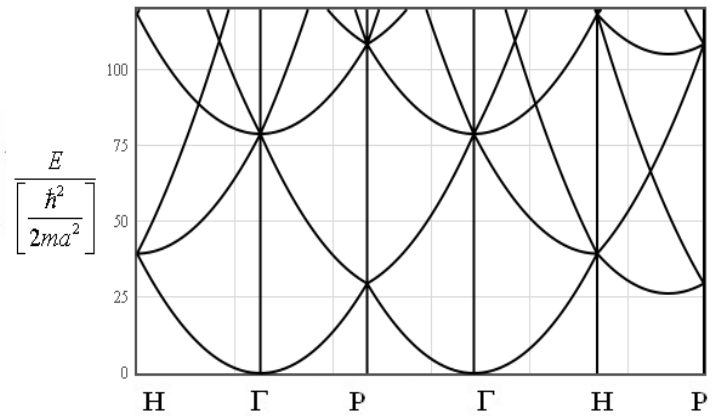
Choose a different order for the symmetry points

Face centered cubic

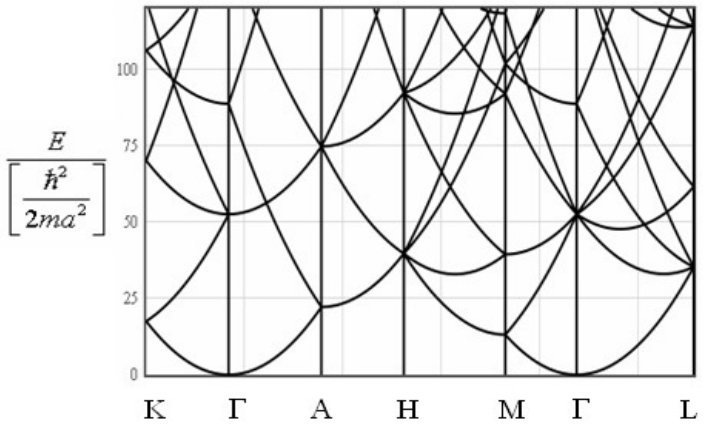


Choose a different order for the symmetry points

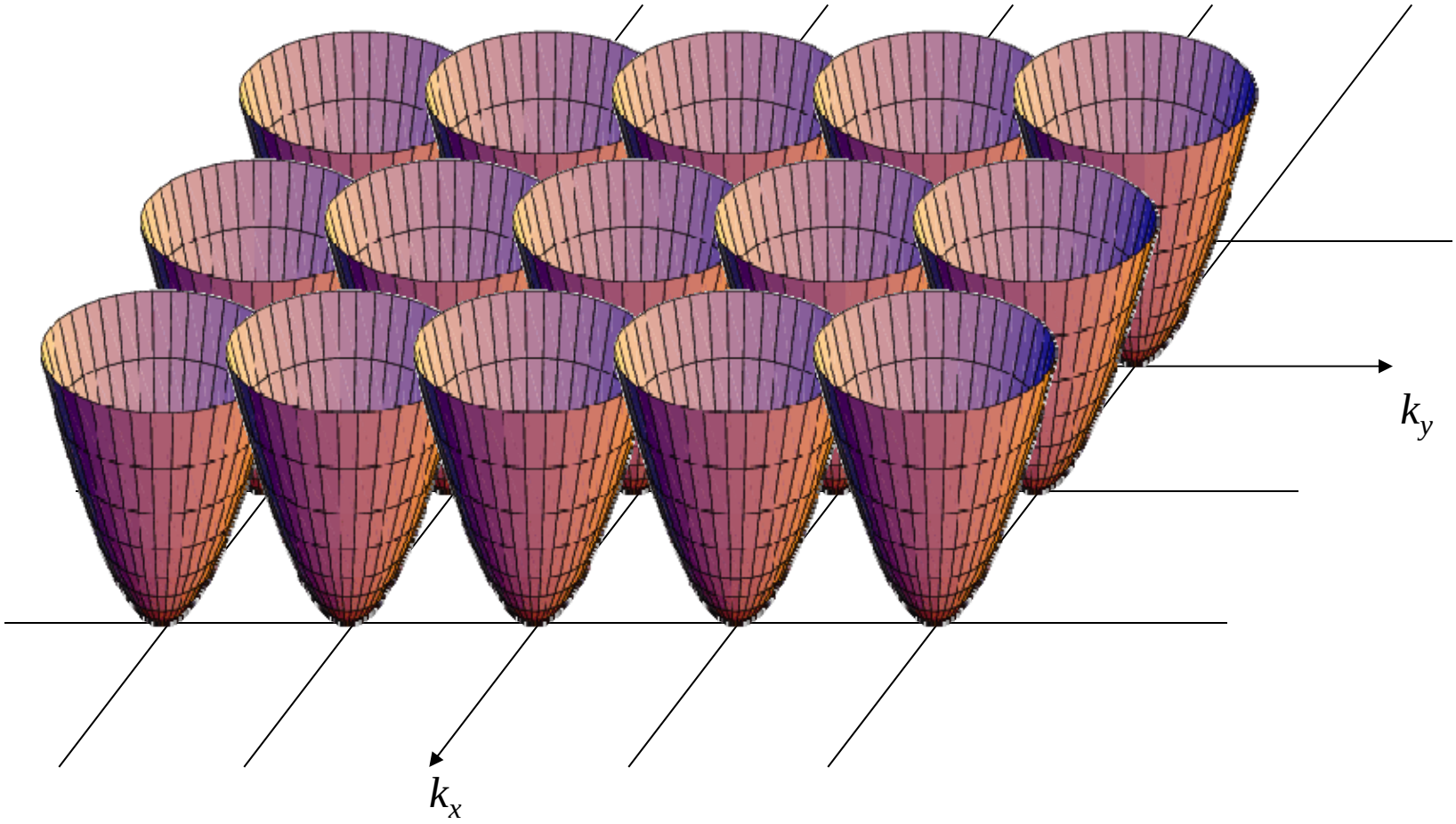
Body centered cubic



Hexagonal

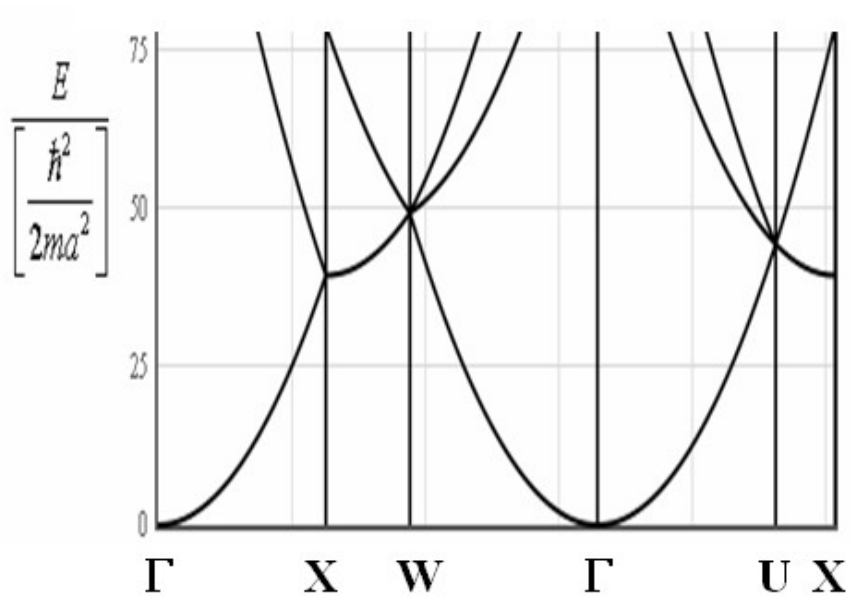


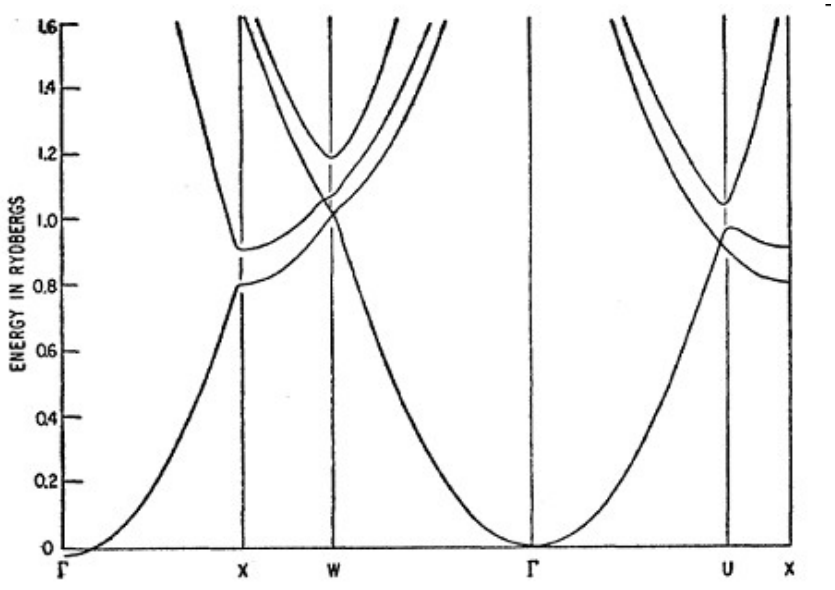
Empty lattice approximation



$$e^{i\vec{k}\cdot\vec{r}} = e^{i\vec{k}'\cdot\vec{r}} e^{i\vec{G}\cdot\vec{r}}$$

Empty lattice approximation





W. Harrison, Phys. Rev. 118 p. 1182 (1960)

aluminum