

Electrons

Review: Electrons

Constructed the grand canonical partition function for noninteracting fermions.

Derived the Fermi-Dirac function.

The thermodynamic properties depend on the density of states.

For free electrons we found the density of states. The free electron model is a two parameter model.

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

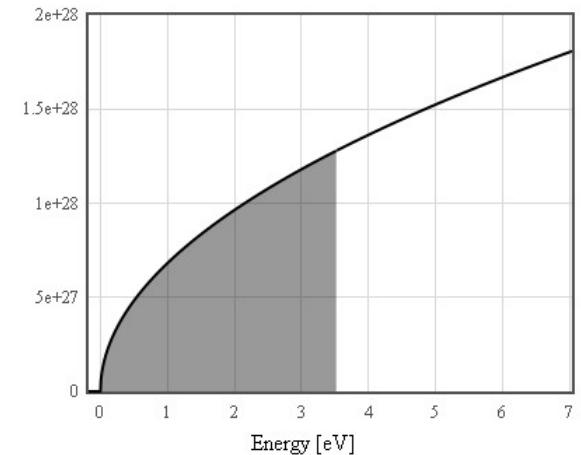
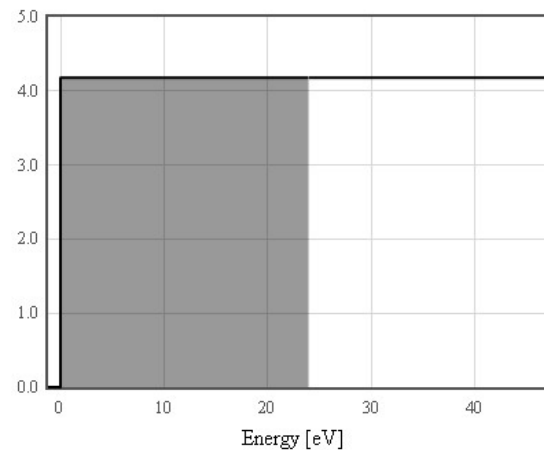
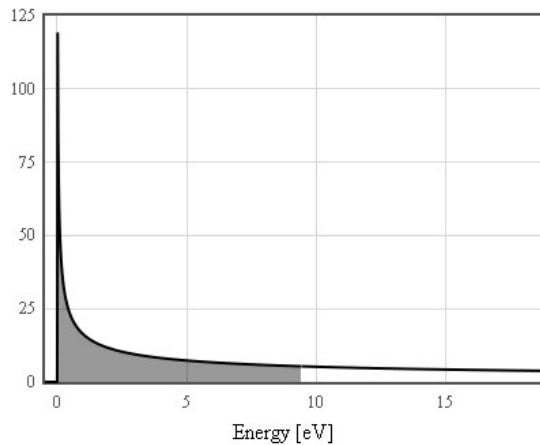
Free electron Fermi gas

$$E = \frac{\hbar^2 k^2}{2m}$$

1 - d $D(k) = \frac{2}{\pi}$ $D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}}$ $\text{J}^{-1}\text{m}^{-1}$

2 - d $D(k) = \frac{k}{\pi}$ $D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F}$ $\text{J}^{-1}\text{m}^{-2}$

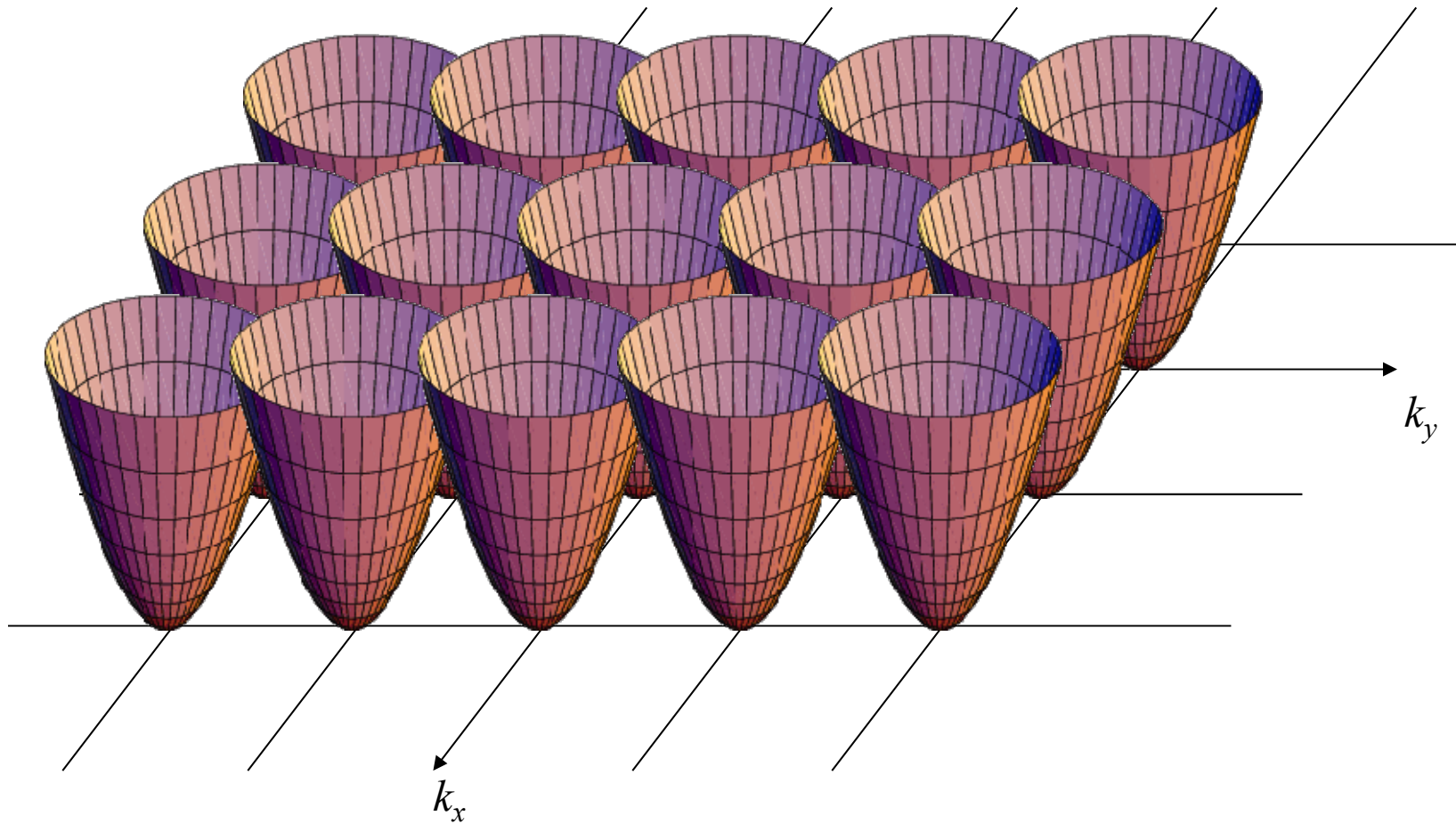
3 - d $D(k) = \frac{k^2}{\pi^2}$ $D(E) = \frac{\pi}{2} \left(\frac{2m}{\hbar^2 \pi^2} \right)^{3/2} \sqrt{E} = \frac{3n}{2E_F^{3/2}} \sqrt{E}$ $\text{J}^{-1}\text{m}^{-3}$



The free electron model is a two parameter model n, m

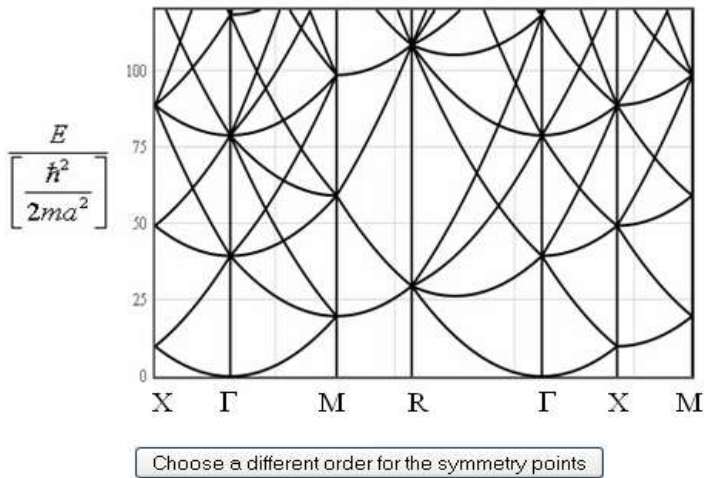
	1-D Schrödinger equation for a free particle $i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}$	2-D Schrödinger equation for a free particle $i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} \right)$	3-D Schrödinger equation for a free particle $i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} \right)$
Eigenfunction solutions	$\psi_k = A_k \exp(i(kx - \alpha t))$	$\psi_k = A_k \exp(i(\vec{k} \cdot \vec{r} - \alpha t))$	$\psi_k = A_k \exp(i(\vec{k} \cdot \vec{r} - \alpha t))$
Eigenvalues of the translation operator $T\psi_k(\vec{r}) = \psi_k(\vec{r} + \vec{R}) = \lambda_k \psi_k(\vec{r})$	$\lambda_k = \exp(ikR)$	$\lambda_{\vec{k}} = \exp(i\vec{k} \cdot \vec{R})$	$\lambda_{\vec{k}} = \exp(i\vec{k} \cdot \vec{R})$
Dispersion relation	$E = \hbar\omega = \frac{\hbar^2 k^2}{2m} \quad \text{J}$	$E = \hbar\omega = \frac{\hbar^2 k^2}{2m} \quad \text{J}$	$E = \hbar\omega = \frac{\hbar^2 k^2}{2m} \quad \text{J}$
Density of states	$D(k) = \frac{2}{\pi}$	$D(k) = \frac{k}{\pi} \quad \text{m}^{-1}$	$D(k) = \frac{k^2}{\pi^2} \quad \text{m}^2$
Density of states $D(E) = D(k) \frac{dk}{dE}$	$D(E) = \frac{1}{\pi\hbar} \sqrt{\frac{2m}{E}} = \frac{n}{2\sqrt{E_F E}} \quad \text{J}^{-1}\text{m}^{-1}$	$D(E) = \frac{m}{\pi\hbar^2} = \frac{n}{E_F} \quad \text{J}^{-1}\text{m}^{-2}$	$D(E) = \frac{(2m)^{3/2}}{2\pi^2\hbar^3} \sqrt{E} = \frac{3n}{2E_F^{3/2}} \sqrt{E} \quad \text{J}^{-1}\text{m}^{-3}$
Fermi energy E_F $n = \int_{-\infty}^{E_F} D(E) dE$	$E_F = \frac{\pi^2 \hbar^2 n^2}{8m} \quad \text{J}$	$E_F = \frac{\pi \hbar^2 n}{m} \quad \text{J}$	$E_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} \quad \text{J}$
$D(E_F)$	$D(E_F) = \frac{4m}{\pi^2 \hbar^2 n} \quad \text{J}^{-1}\text{m}^{-1}$	$D(E_F) = \frac{m}{\pi \hbar^2} \quad \text{J}^{-1}\text{m}^{-2}$	$D(E_F) = \frac{m(3n)^{1/3}}{\pi^3 \hbar^2} \quad \text{J}^{-1}\text{m}^{-3}$
$D'(E_F) = \frac{dD}{dE} \Big _{E=E_F}$	$D'(E_F) = \frac{-16m^2}{\pi^4 \hbar^4 n^3} \quad \text{J}^2\text{m}^{-1}$	$D'(E_F) = 0 \quad \text{J}^2\text{m}^{-2}$	$D'(E_F) = \frac{m^2}{\hbar^4 \sqrt[3]{3\pi^8 n}} \quad \text{J}^2\text{m}^{-3}$
Chemical potential μ $n = \int_{-\infty}^{\mu} D(E) f(E) dE$	$\mu \approx E_F - \frac{\pi^2}{6} (k_B T)^2 \frac{D'(E_F)}{D(E_F)} \quad \text{J}$ $\approx \frac{\pi^2 \hbar^2 n^2}{8m} + \frac{2m}{3\hbar^2 n^2} (k_B T)^2 \quad \text{J}$	$\mu = k_B T \ln \left(\exp \left(\frac{E_F}{k_B T} \right) - 1 \right) \quad \text{J}$ $= k_B T \ln \left(\exp \left(\frac{\pi \hbar^2 n}{m k_B T} \right) - 1 \right) \quad \text{J}$	$\mu \approx E_F - \frac{\pi^2}{6} (k_B T)^2 \frac{D'(E_F)}{D(E_F)} \quad \text{J}$ $\approx \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} - \frac{\pi^2 m}{2\hbar^2 3^{10/3} n^{1/3}} (k_B T)^2 \quad \text{J}$
Internal energy distribution $u(E) = E \frac{D(E)}{\exp \left(\frac{E - \mu}{k_B T} \right) + 1}$	$u(E) = \frac{n}{2} \sqrt{\frac{E}{E_F}} \frac{1}{\exp \left(\frac{E - \mu}{k_B T} \right) + 1} \quad \text{m}^{-1}$ $= \frac{1}{\pi \hbar} \sqrt{2mE} \frac{1}{(E - \mu)} \quad \text{m}^{-1}$	$u(E) = \frac{n}{E_F} \frac{E}{\exp \left(\frac{E - \mu}{k_B T} \right) + 1} \quad \text{m}^{-2}$ $= \frac{m}{\pi \hbar^2} \frac{E}{(E - \mu)} \quad \text{m}^{-2}$	$u(E) = \frac{3n}{2} \left(\frac{E}{E_F} \right)^{3/2} \frac{1}{\exp \left(\frac{E - \mu}{k_B T} \right) + 1} \quad \text{m}^{-3}$ $= \frac{1}{2\pi^2 \hbar^3} (2mE)^{3/2} \quad \text{m}^{-3}$

Empty lattice approximation

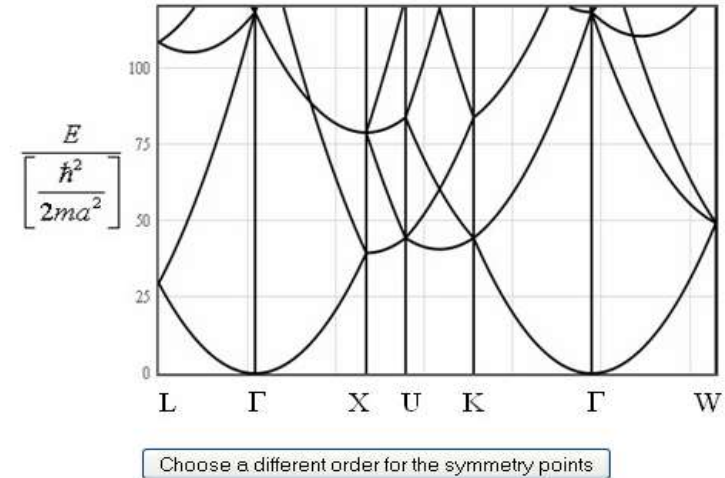


Empty lattice approximation

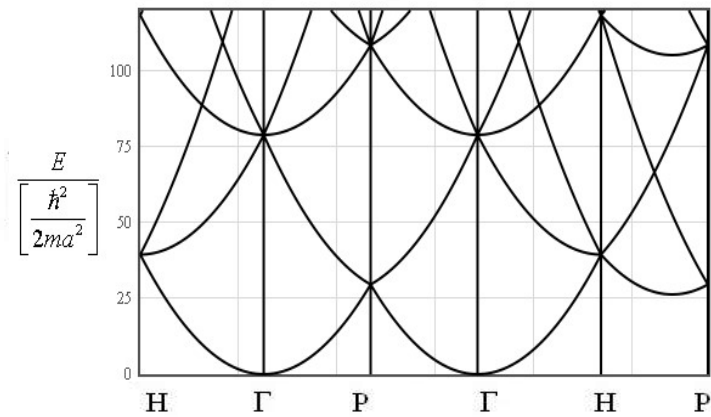
Simple cubic



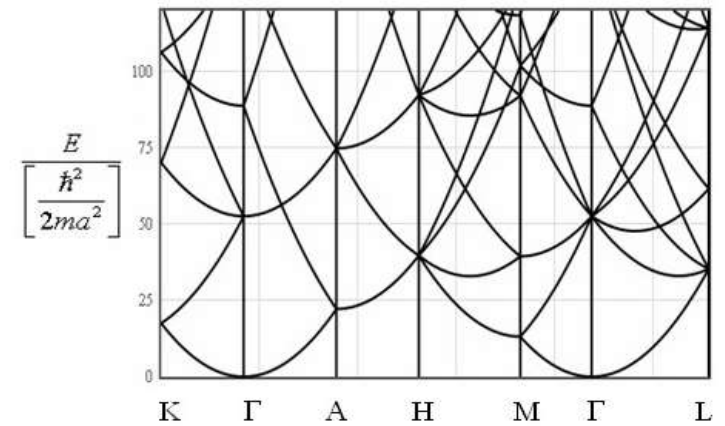
Face centered cubic



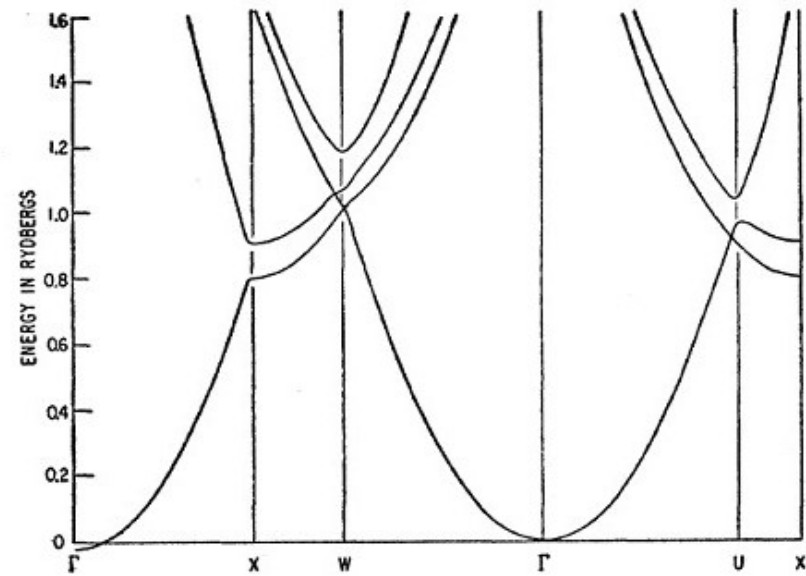
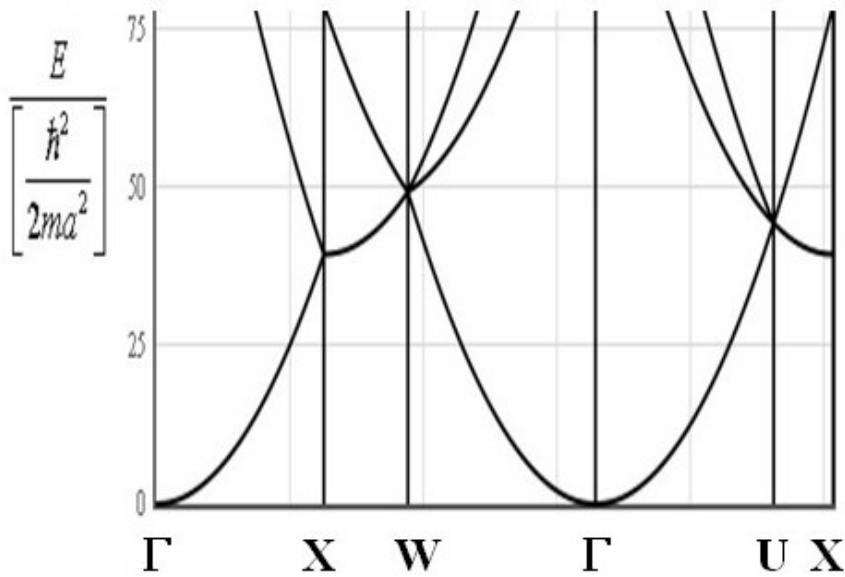
Body centered cubic



Hexagonal



Empty lattice approximation



aluminum

2N states per Brillouin zone

A crystal $L \times L \times L$ has $N = \frac{L^3}{a^3}$ unit cells.

The first Brillouin zone contains $N = \frac{\left(\frac{2\pi}{a}\right)^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{L^3}{a^3}$ k points.

Each k state can hold 2 electrons (spin).

There are $2N$ states per Brillouin zone.

There are N translational symmetries.

The N translational symmetries

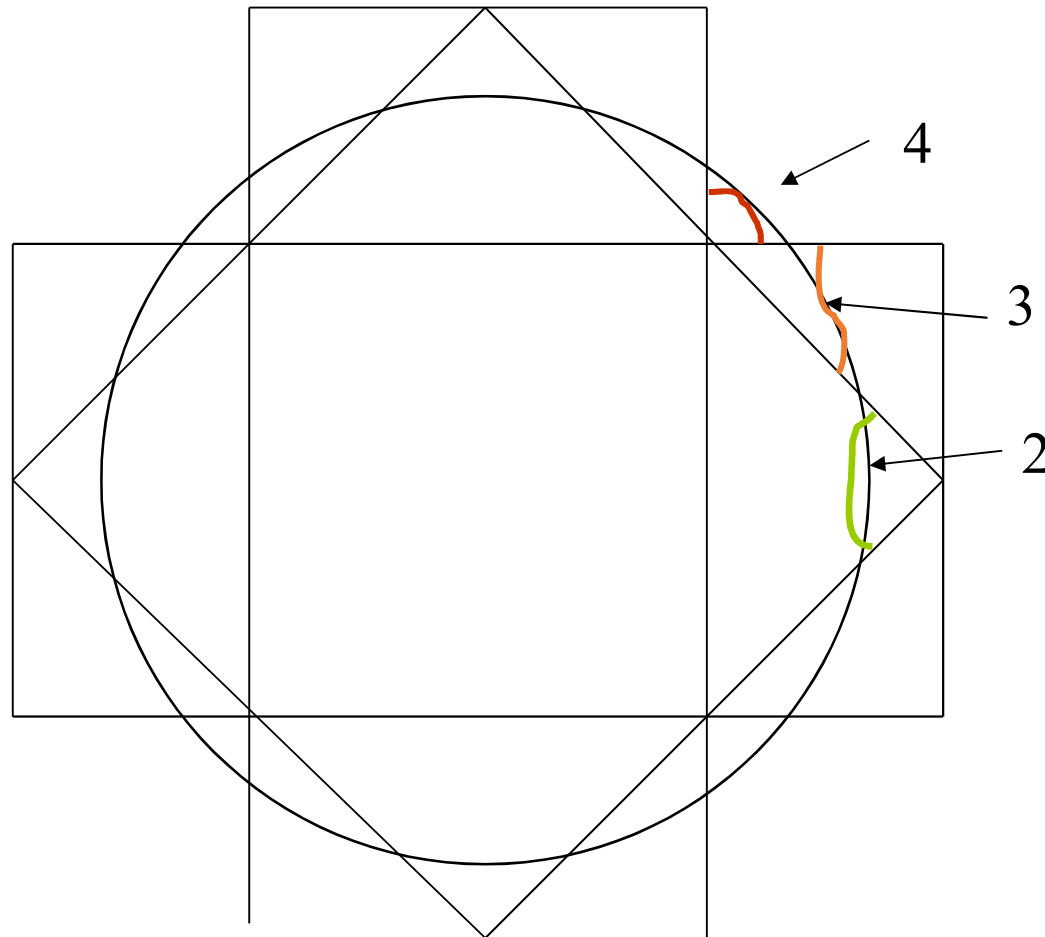
A crystal $L \times L \times L$ has $N = \frac{L^3}{a^3}$ unit cells.

$$T_{mnl} e^{i\vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot (\vec{r} + m\vec{a}_1 + n\vec{a}_2 + l\vec{a}_3)} u_{\vec{k}}(\vec{r} + m\vec{a}_1 + n\vec{a}_2 + l\vec{a}_3) = e^{i\vec{k} \cdot (m\vec{a}_1 + n\vec{a}_2 + l\vec{a}_3)} e^{i\vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r})$$

$$m, n, l = -\frac{L}{2a}, \dots, 2-, -1, 0, 1, 2, \dots, \frac{L}{2a}$$

$$k_x, k_y, k_z = -\frac{2\pi}{a}, \dots, -\frac{4\pi}{L}, -\frac{2\pi}{L}, 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \dots, \frac{2\pi}{a}$$

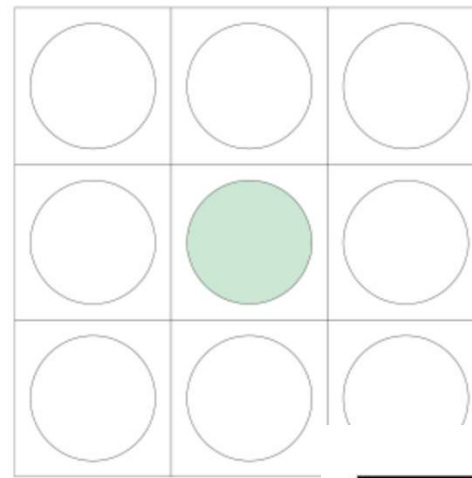
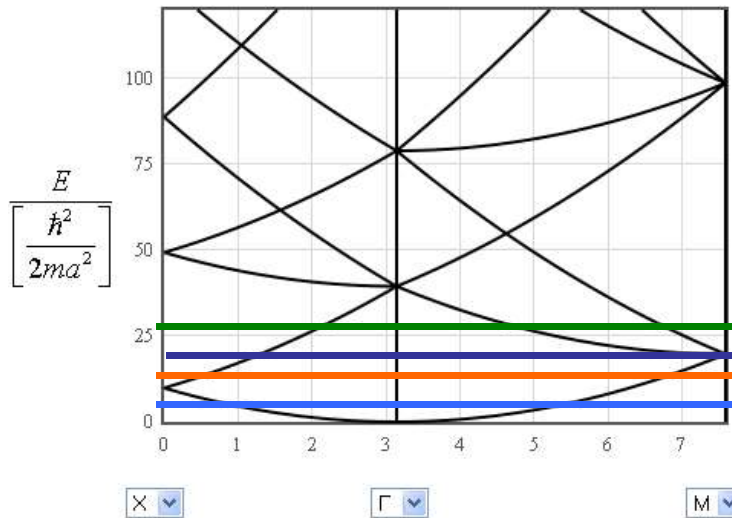
Constructing Fermi surface



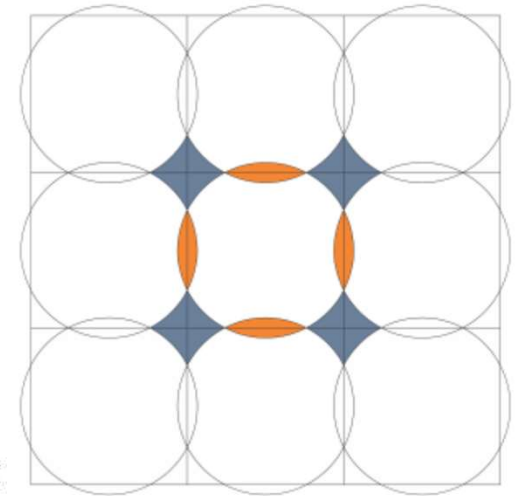
No Fermi surface in the 1st Brillouin zone

2d square

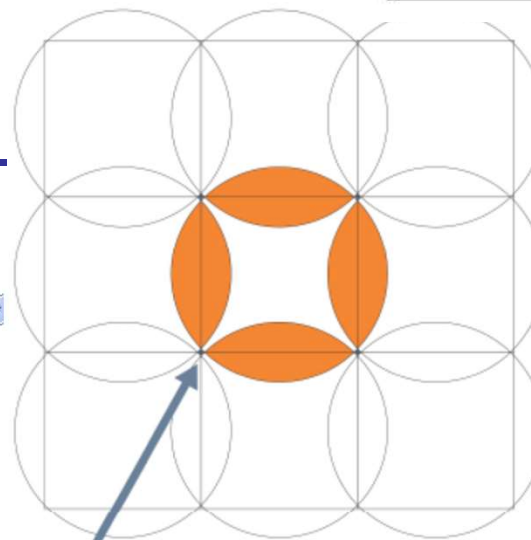
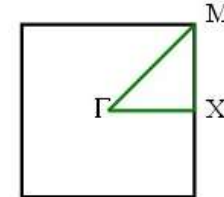
$2N$ electron states in a Brillouin zone



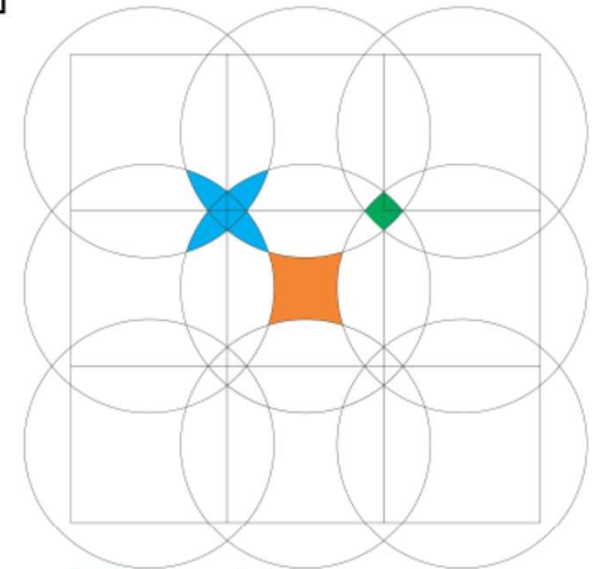
1st zone electrons



1st zone holes
2nd zone electrons



1st zone holes
2nd zone electrons



2nd zone holes
3rd zone electrons
4th zone electrons

The Fermi surface strikes the Brillouin zone boundary at 90° .