The N translational symmetries

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

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

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

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

Multiply by $\frac{L}{2\pi}$

$$\frac{L}{2\pi}k_x,\frac{L}{2\pi}k_y,\frac{L}{2\pi}k_z = -\frac{L}{2a},\cdots,-2,-1,0,1,2,\cdots,\frac{L}{2a}$$

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 one parameter model.

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

Free electron Fermi gas 1-d

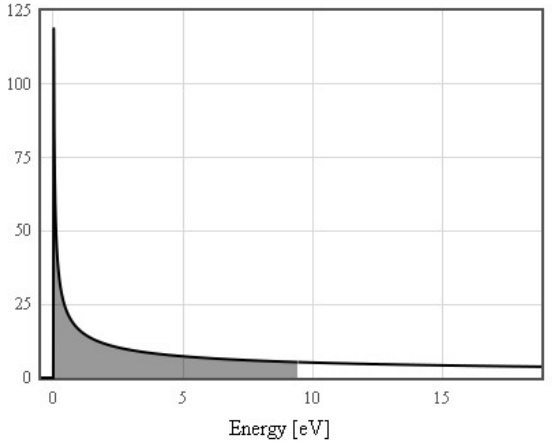
$$D(k) = \frac{2}{\pi}$$

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

$$dk = \frac{m}{\hbar^2 k} dE = \frac{1}{\hbar}\sqrt{\frac{m}{2E}} dE$$

$$D(k)dk = D(E)dE$$

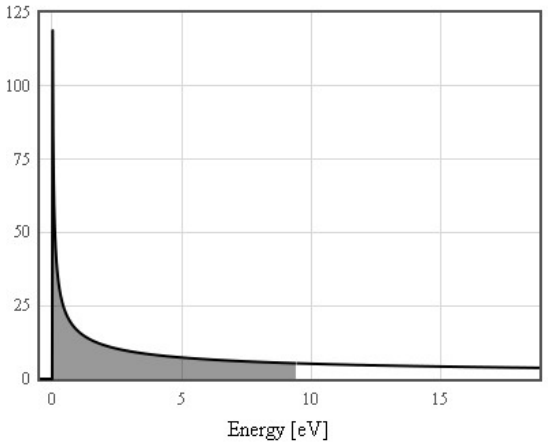
$$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \qquad \mathrm{J^{-1}m^{-1}}$$

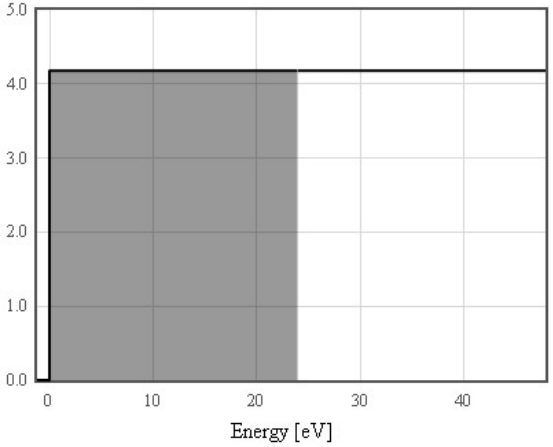


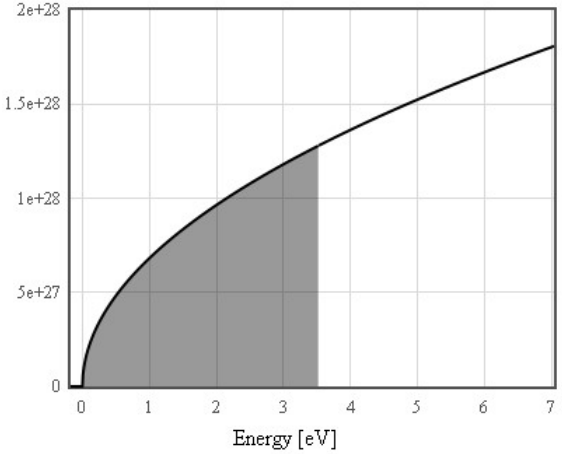
Free electron Fermi gas

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

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







The free electron model is a one parameter model

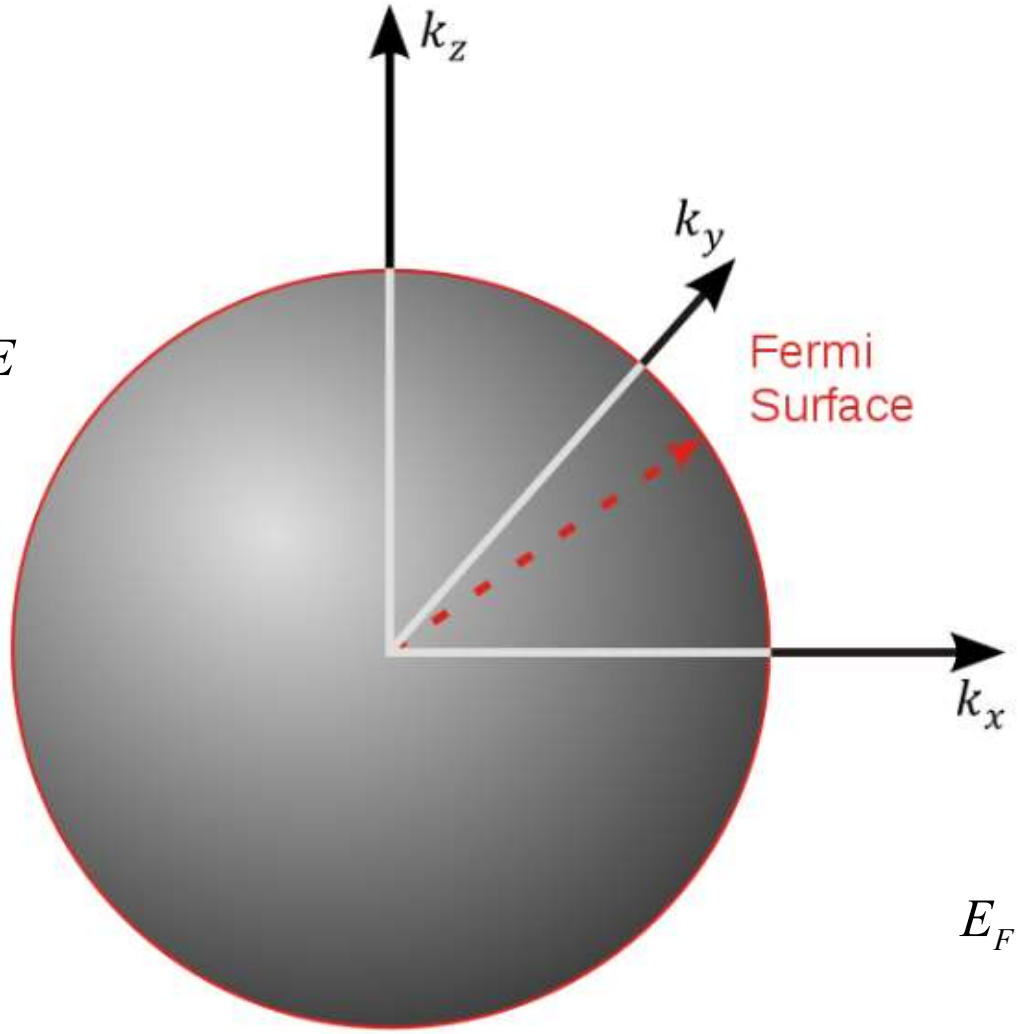
	1-D Schrödinger equation for a free particle $i\hbar\frac{d\psi}{dt}=-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$	2-D Schrödinger equation for a free particle $i\hbar\frac{d\psi}{dt}=-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}\right)$	3-D Schrödinger equation for a free particle $i\hbar\frac{d\psi}{dt}=-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{d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

Fermi surface for free electrons

$$n = \int_{-\infty}^{E_F} D(E)dE$$

$$n = \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\int_{-\infty}^{E_F}\sqrt{E}dE$$

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{\frac{2}{3}}$$

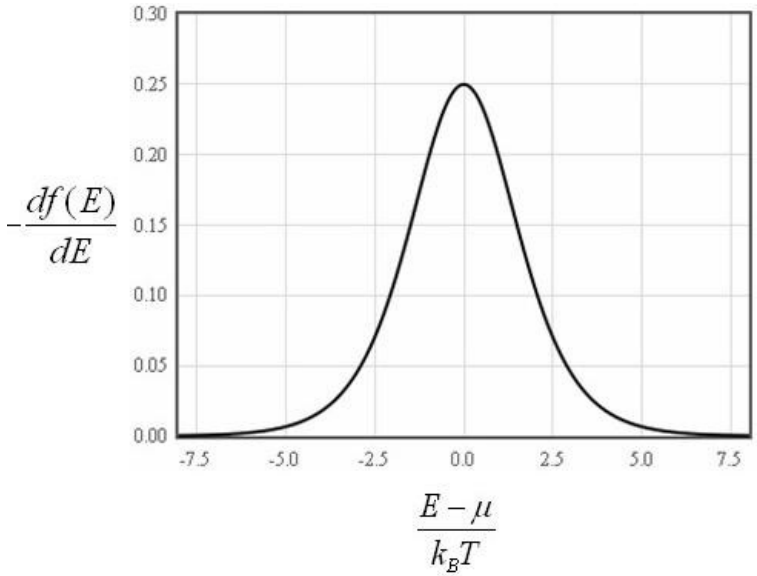


$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

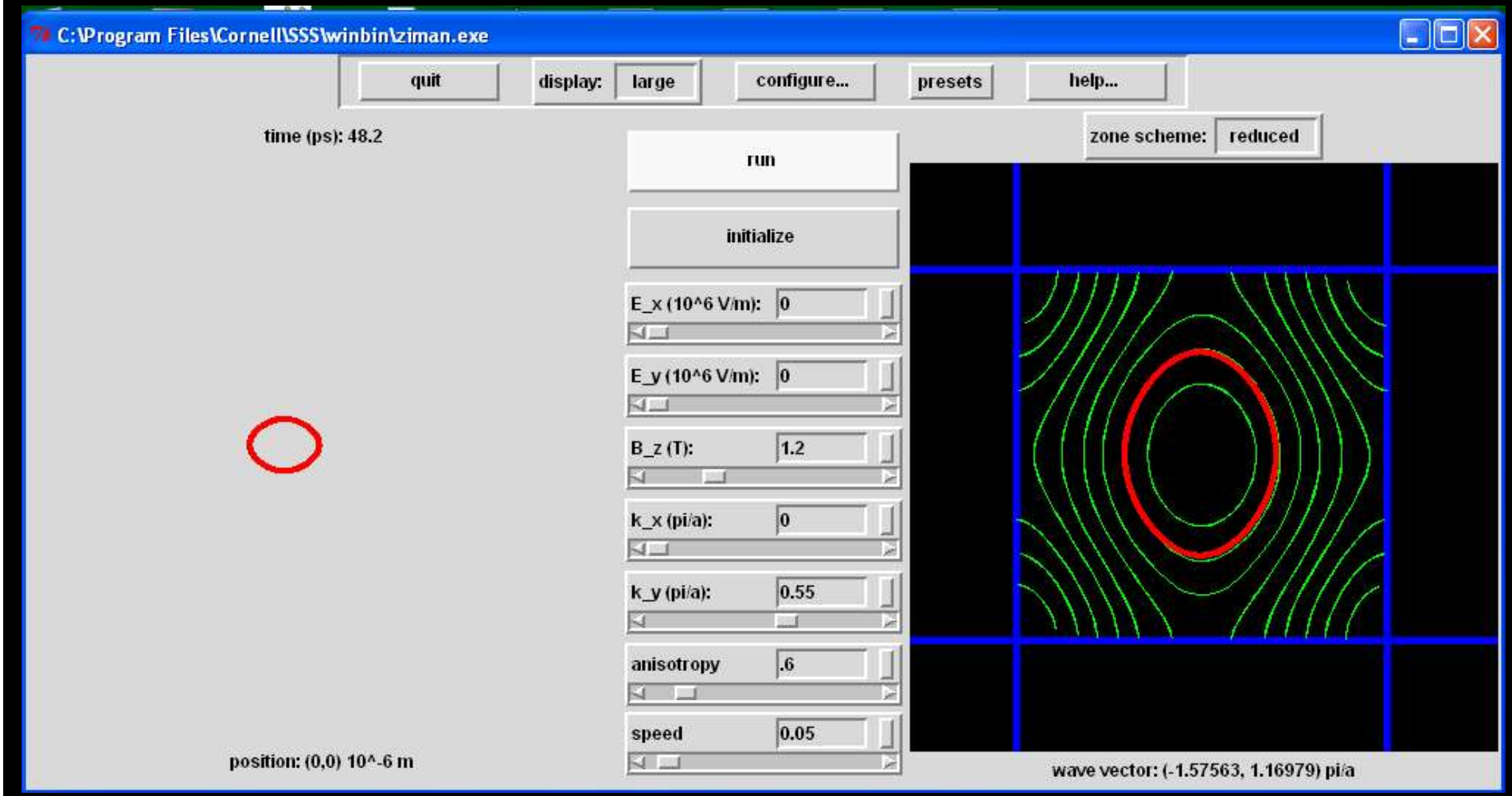
Properties of metals depend mostly on the electron states at the Fermi surface

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

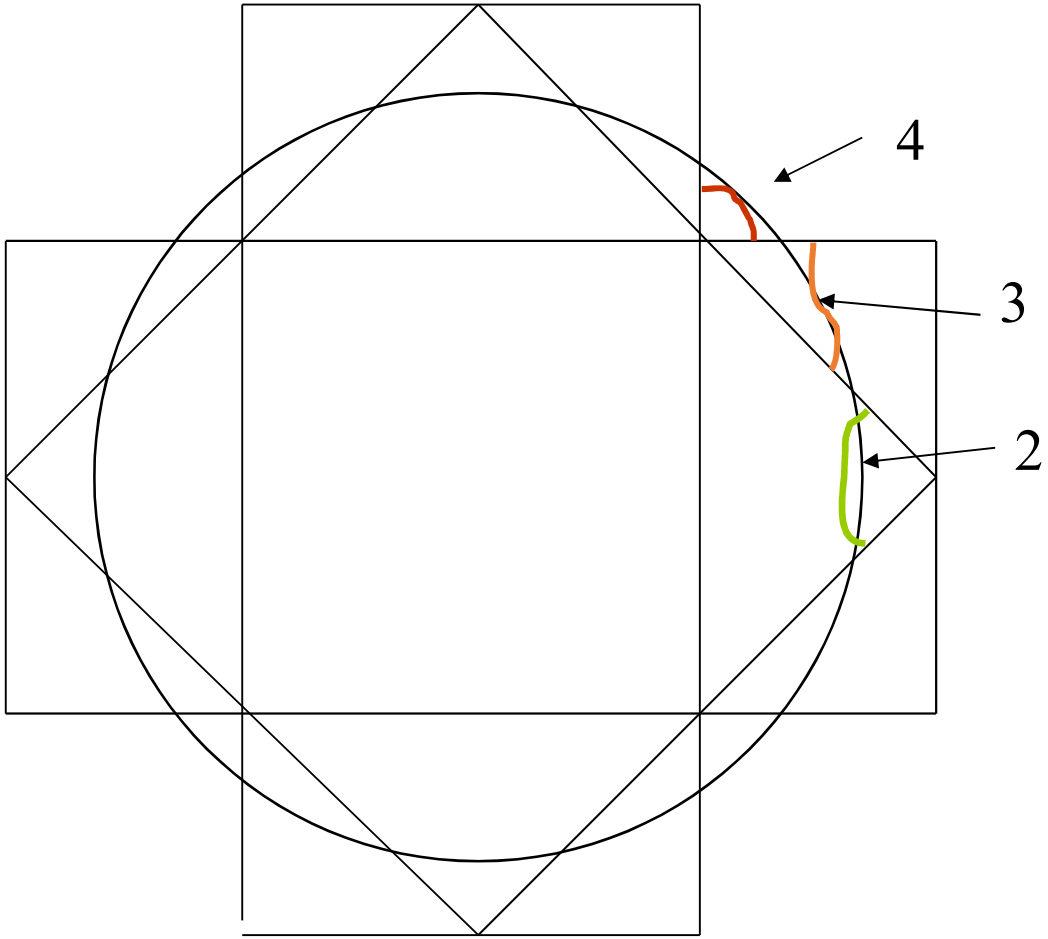
$$n = \int_{-\infty}^{\infty} D(E) f(E) dE = K(\infty) f(\infty) - K(-\infty) f(-\infty) - \int_{-\infty}^{\infty} K(E) \frac{f(E)}{dE} dE.$$



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


C:\Program Files\Cornell\SSS\winbin\ziman.exe
quit
display:
large
configure...
presets
help...
time (ps): 48.2
run
initialize
zone scheme:
reduced
E_x (10^6 V/m):
0
E_y (10^6 V/m):
0
B_z (T):
1.2
k_x (pi/a):
0
k_y (pi/a):
0.55
anisotropy
.6
speed
0.05
position: (0,0) 10^-6 m
wave vector: (-1.57563, 1.16979) pi/a

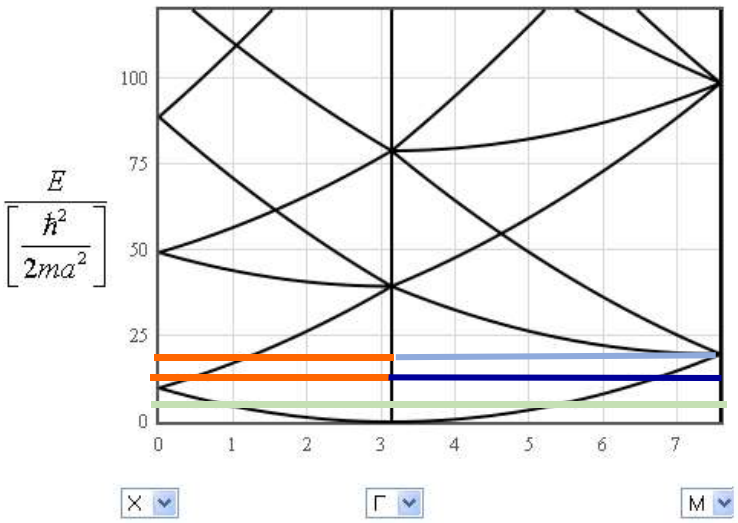
Constructing Fermi surface

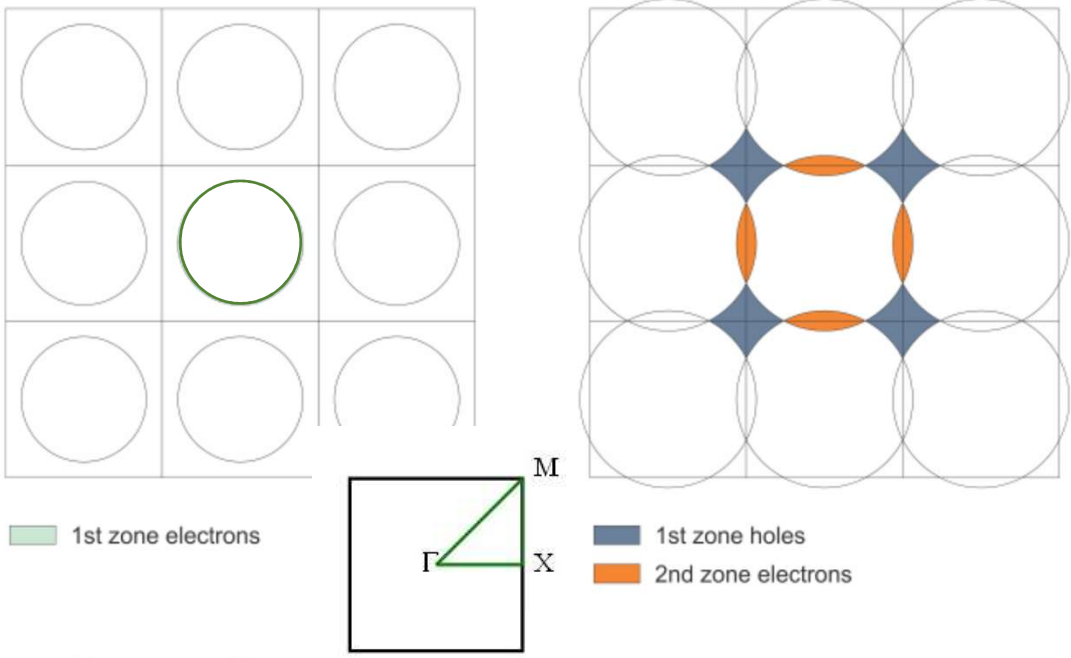


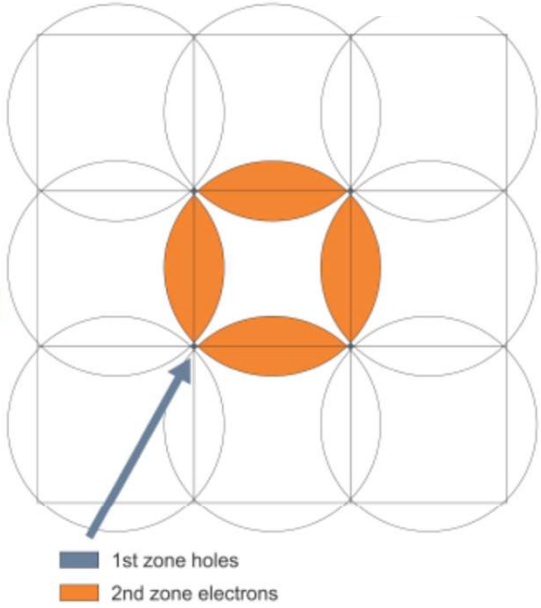
No Fermi surface in the 1st Brillouin zone

2d square

$2N$ electron states in a Brillouin zone

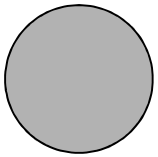




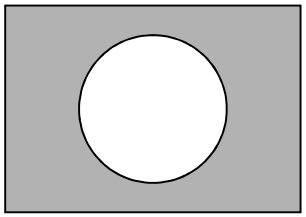


The Fermi surface strikes the Brillouin zone boundary at 90°.

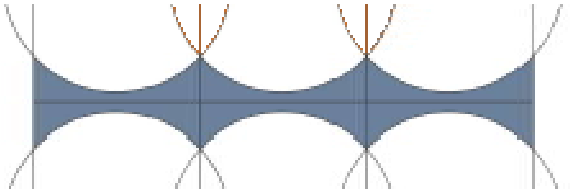
2d rectangular



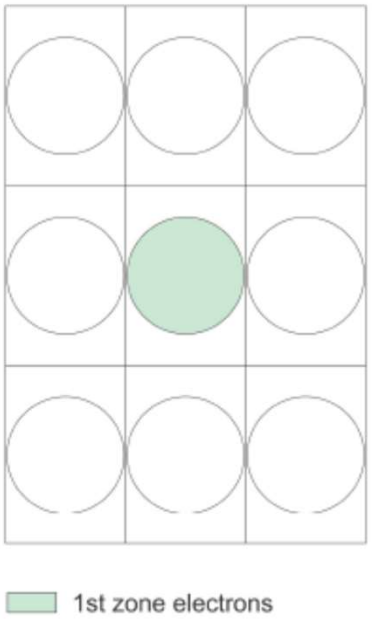
electron orbits
enclose filled states

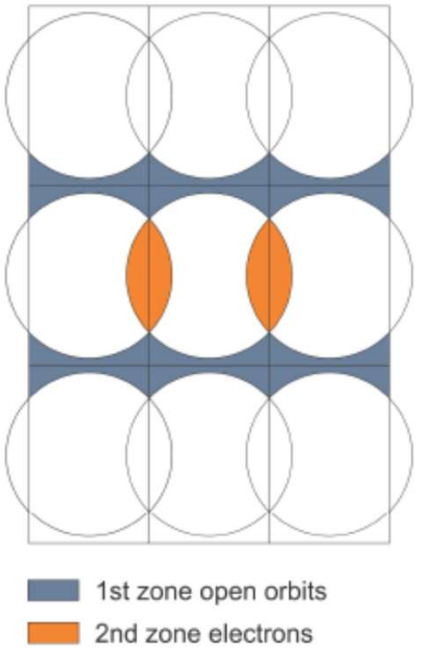


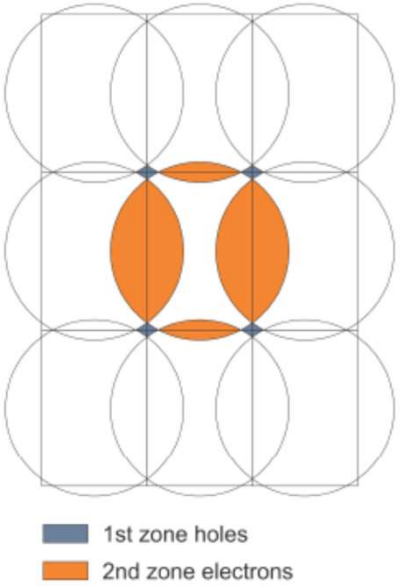
hole orbits
enclose empty states



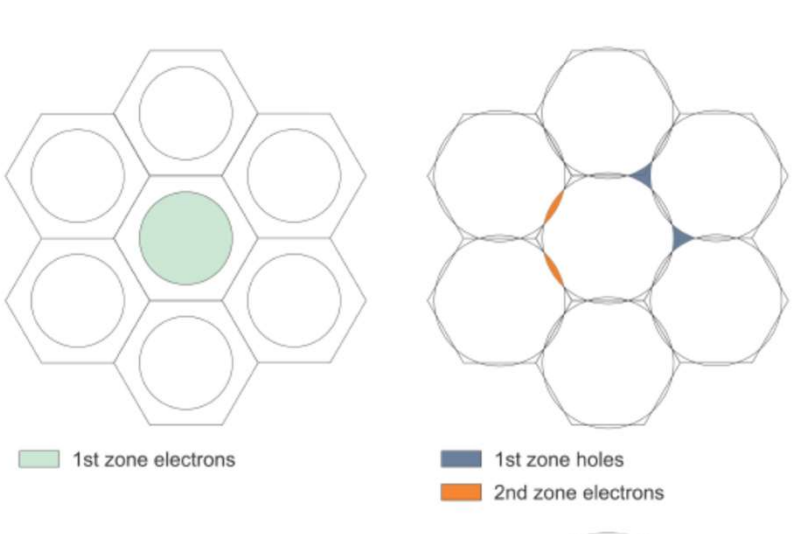
open orbits



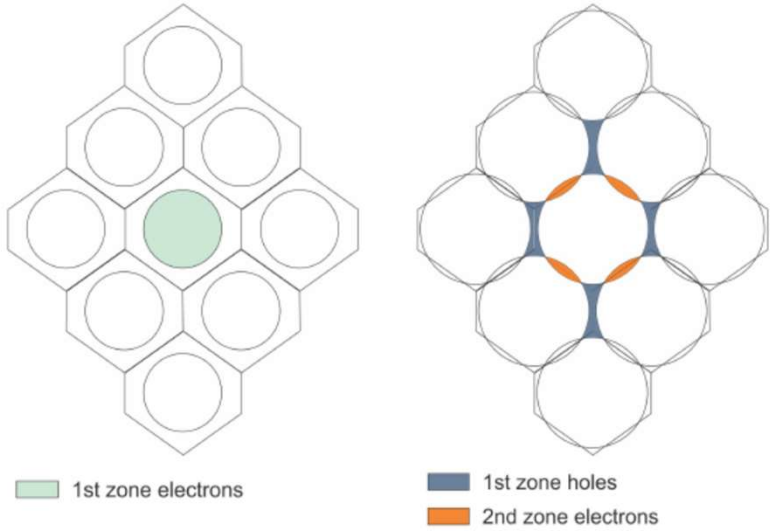




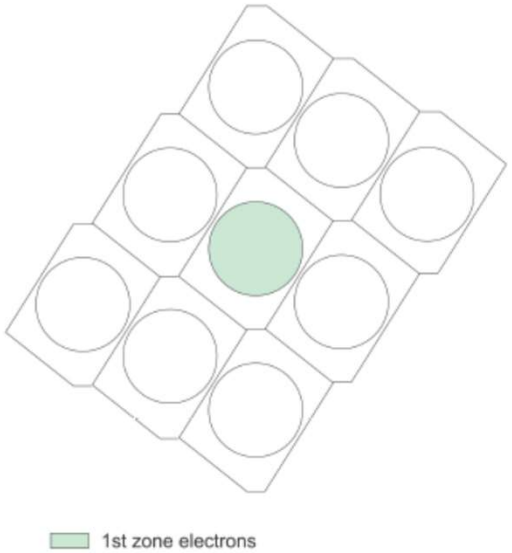
2d hexagonal

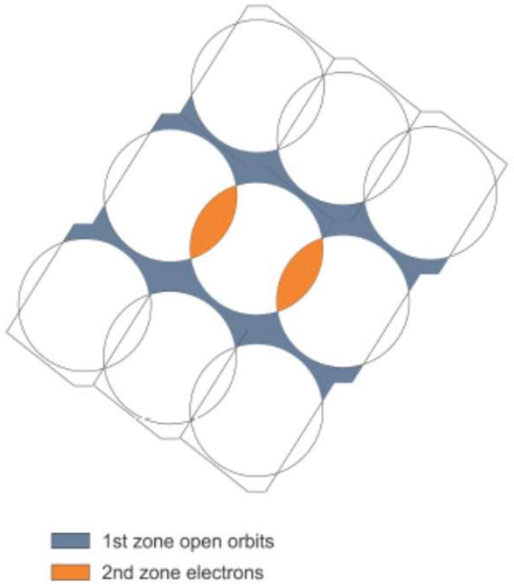


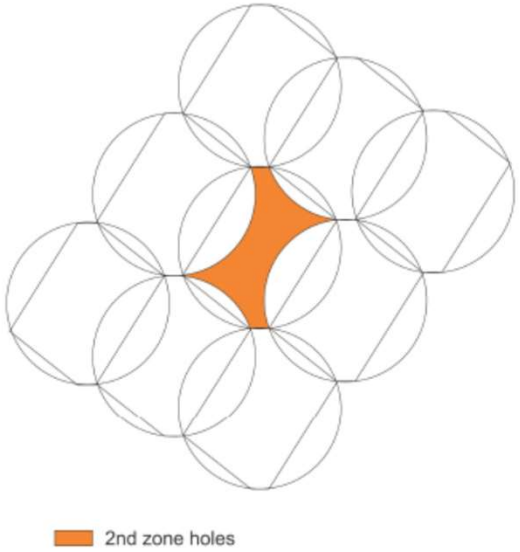
2d centered rectangular



2d oblique


1st zone electrons


1st zone open orbits
2nd zone electrons

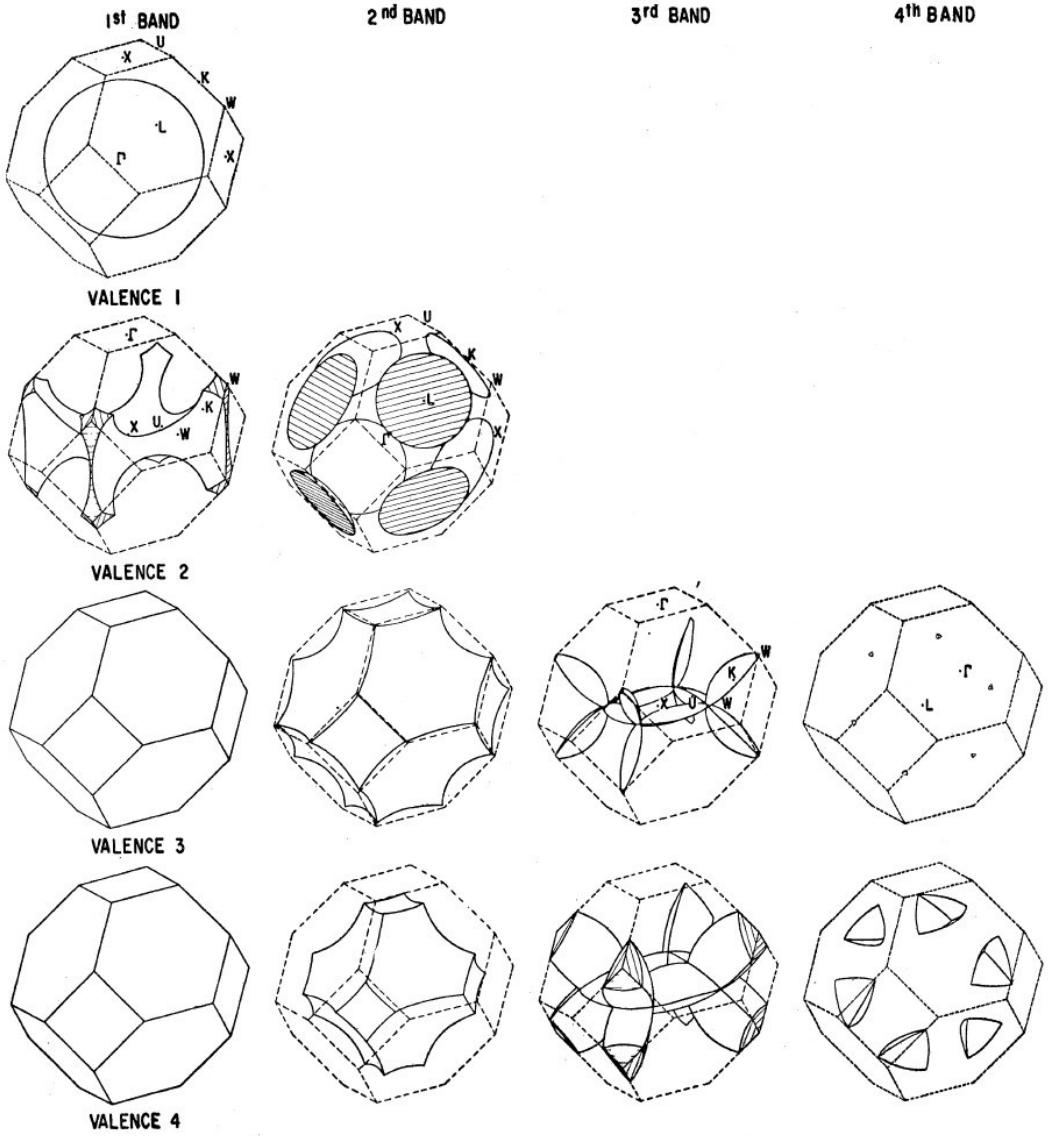

2nd zone holes

Student project

Replot the Fermi surfaces in 2-D plotting just the surface.

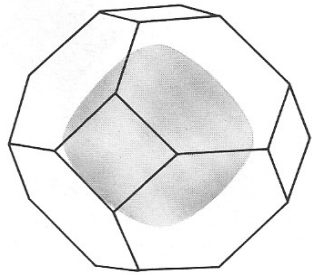
It would be best if we use a program to draw the Fermi surfaces dynamically.

Fermi surface for fcc in the empty lattice approximation

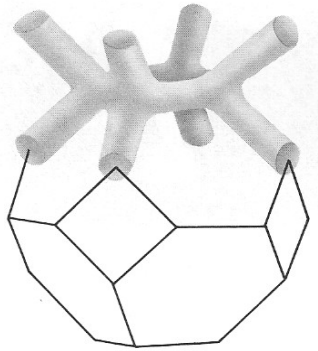


Valence 4

2nd zone holes



3rd zone monster



4th zone electrons