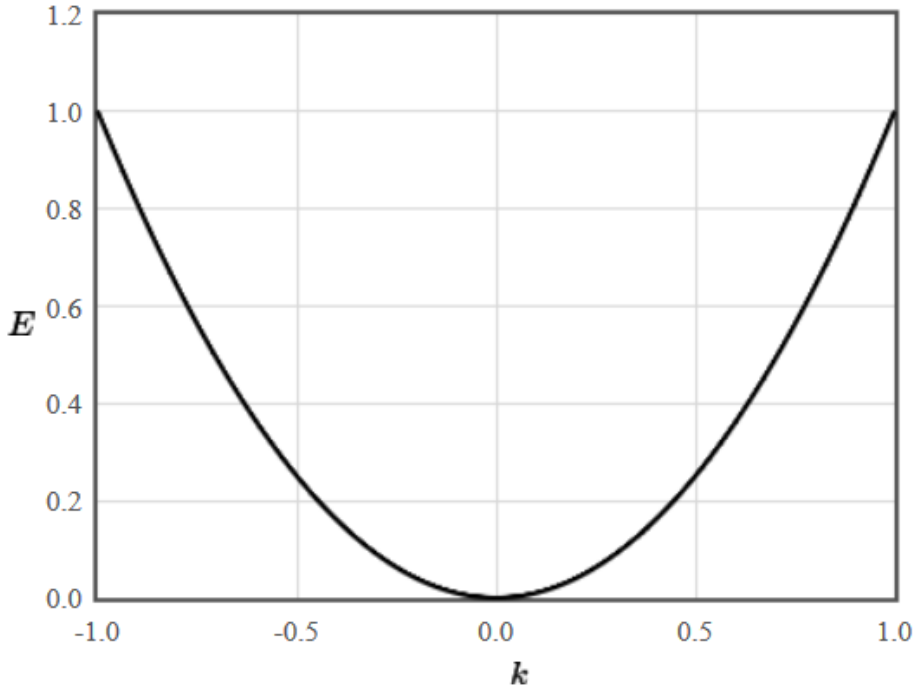
Empty lattice approximation

Empty lattice approximation

Free electrons cannot absorb photons



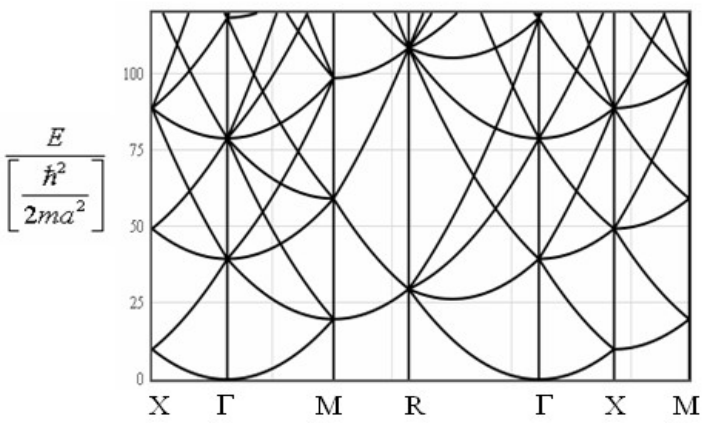
$$\hbar\vec{k}_f = \hbar\vec{k}_i + \hbar\vec{G}$$

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

Laue condition

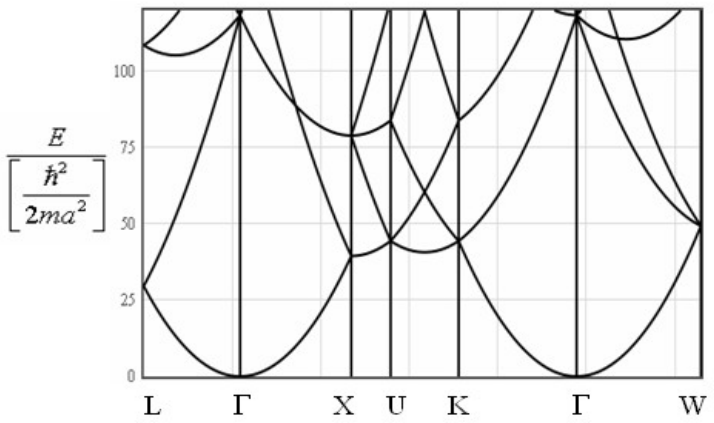
Empty lattice approximation

Simple cubic



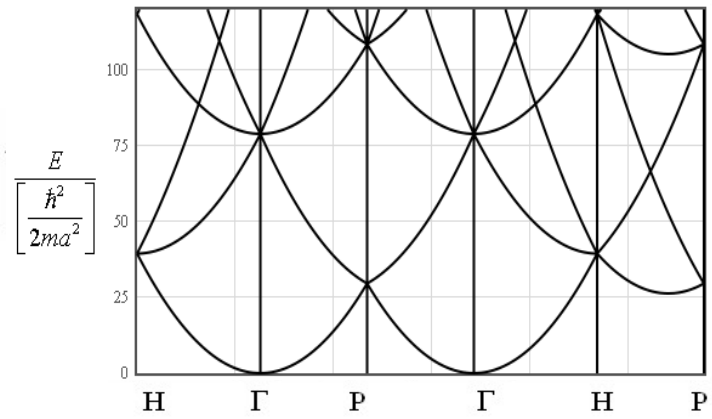
Choose a different order for the symmetry points

Face centered cubic

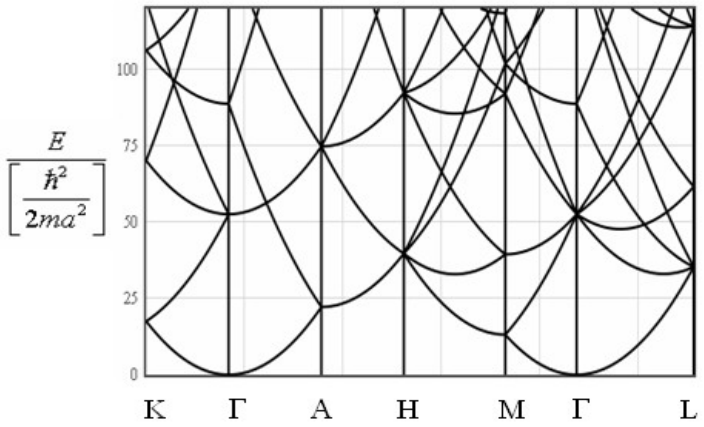


Choose a different order for the symmetry points

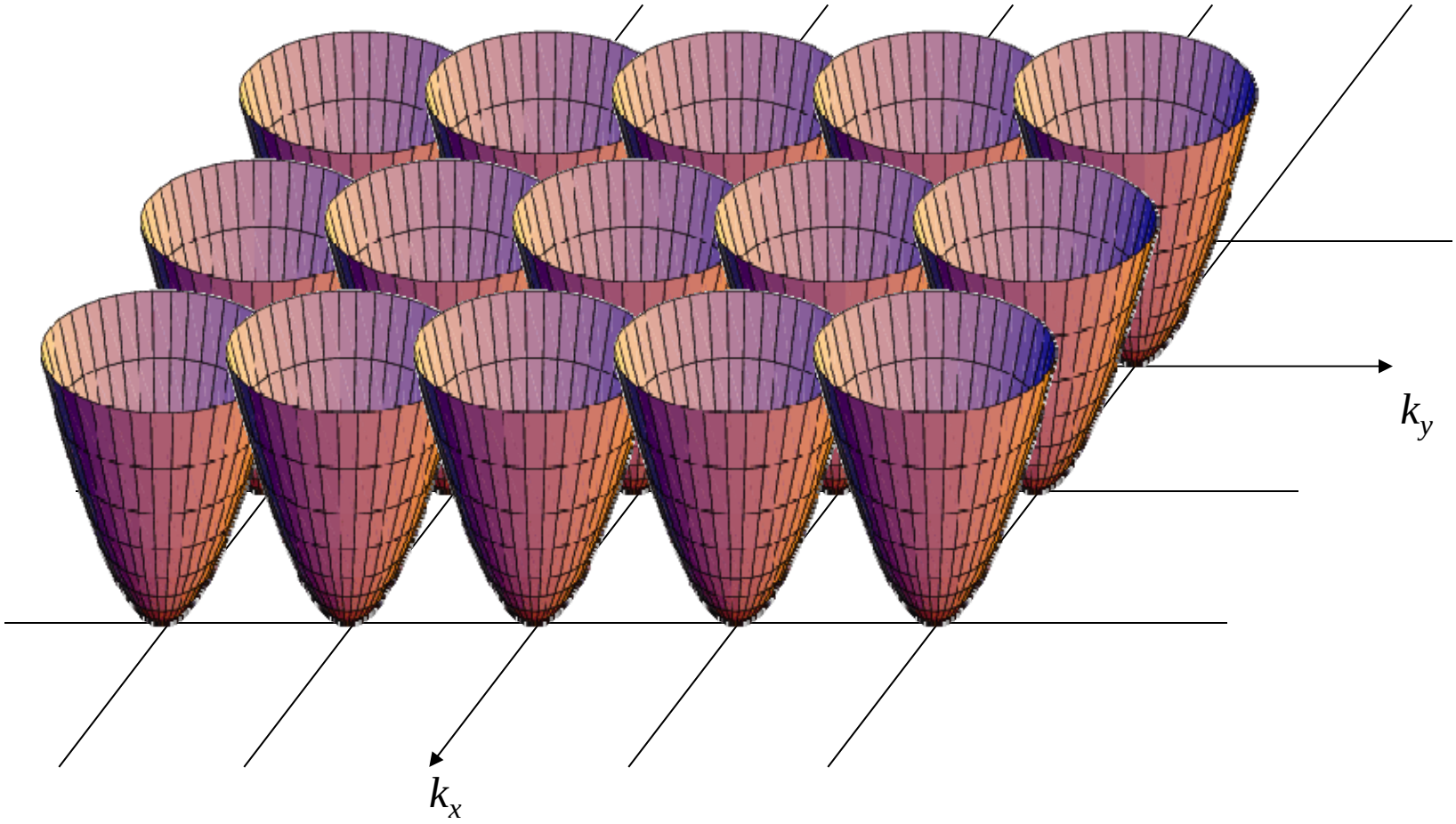
Body centered cubic



Hexagonal

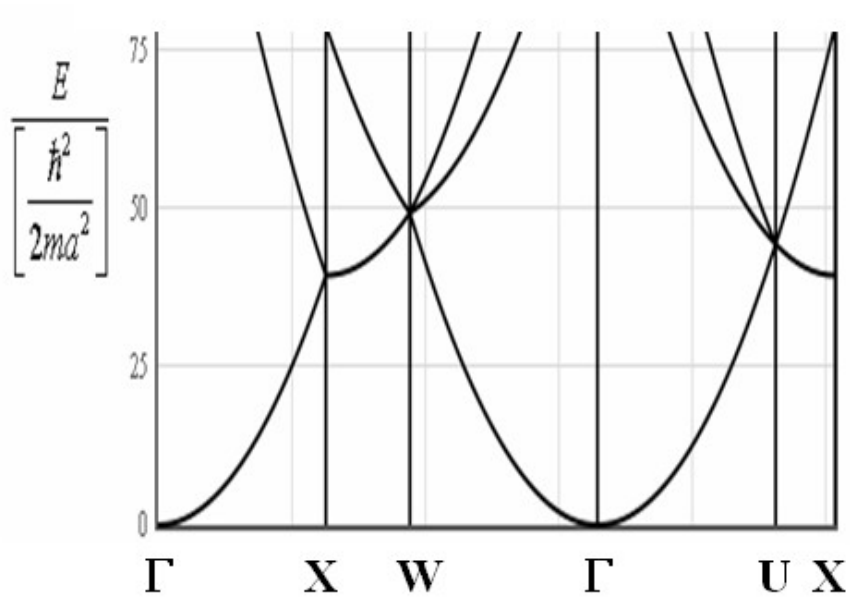


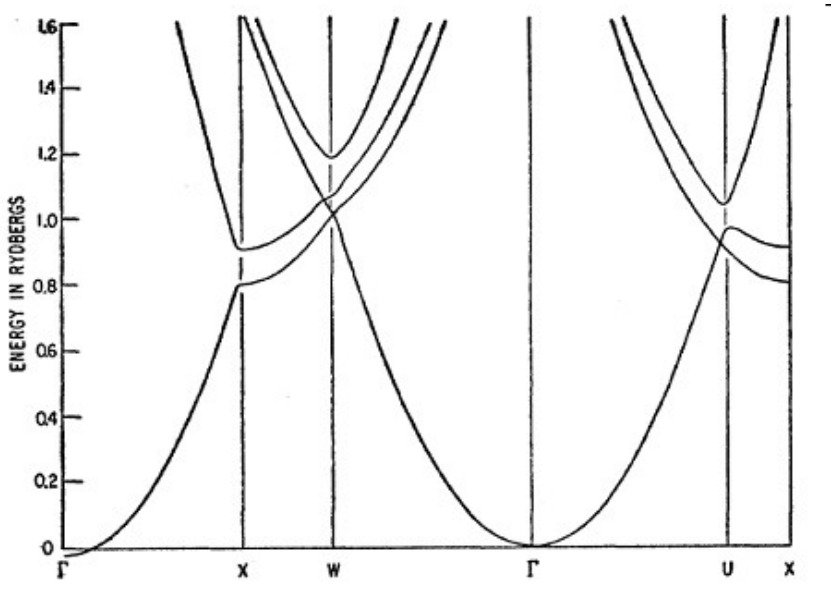
Empty lattice approximation



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

Empty lattice approximation

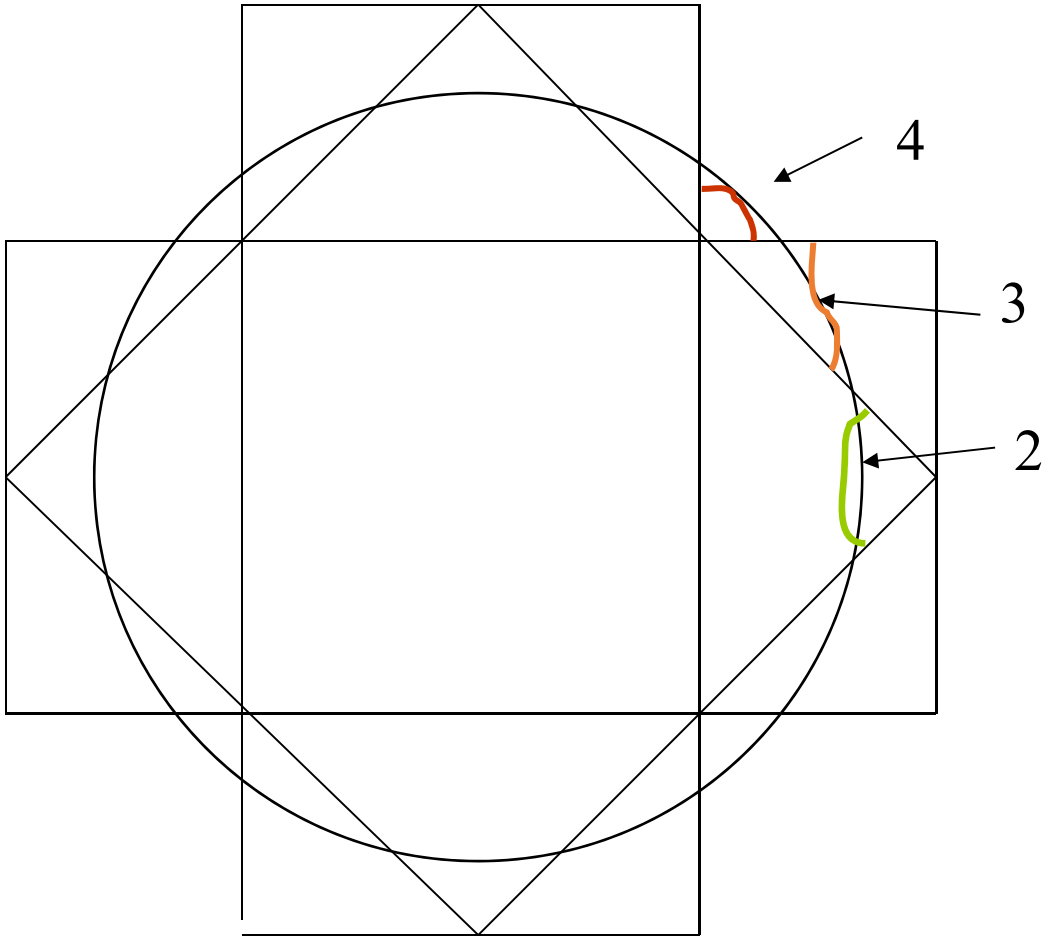




W. Harrison, Phys. Rev. 118 p. 1182 (1960)

aluminum

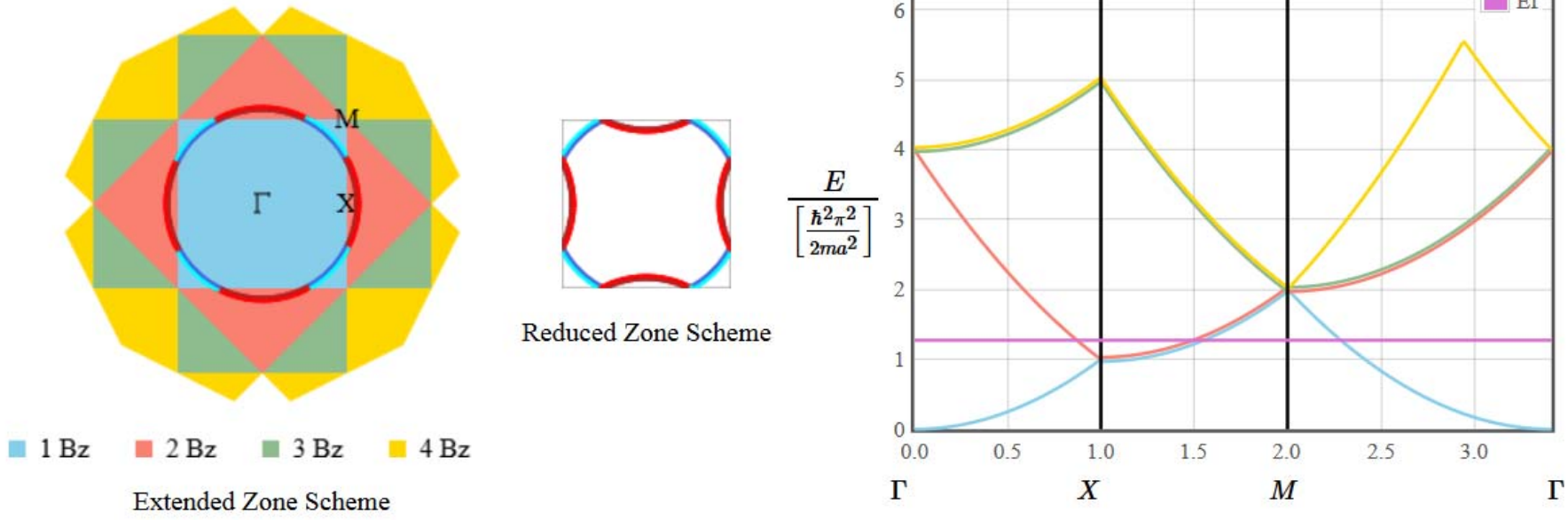
Constructing Fermi surface



No Fermi surface in the 1st Brillouin zone

2d square lattice

2*N* electron states in a Brillouin zone



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

http://lampx.tugraz.at/~hadley/ss2/fermisurface/2d_fermisurface/2dsquare.php

Brillouin zones of two-dimensional Bravais lattices

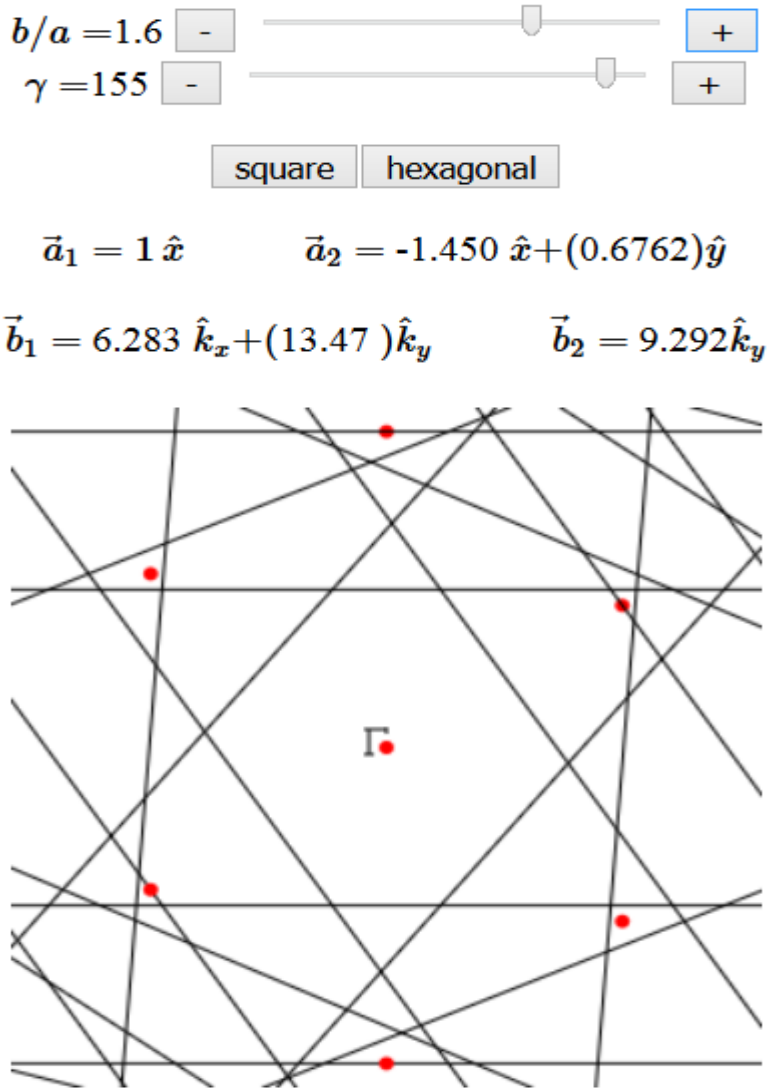
$$\vec{a}_1 = a\,\hat{x}, \qquad \vec{a}_2 = b\cos\gamma\,\hat{x} + b\sin\gamma\,\hat{y}.$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}.$$

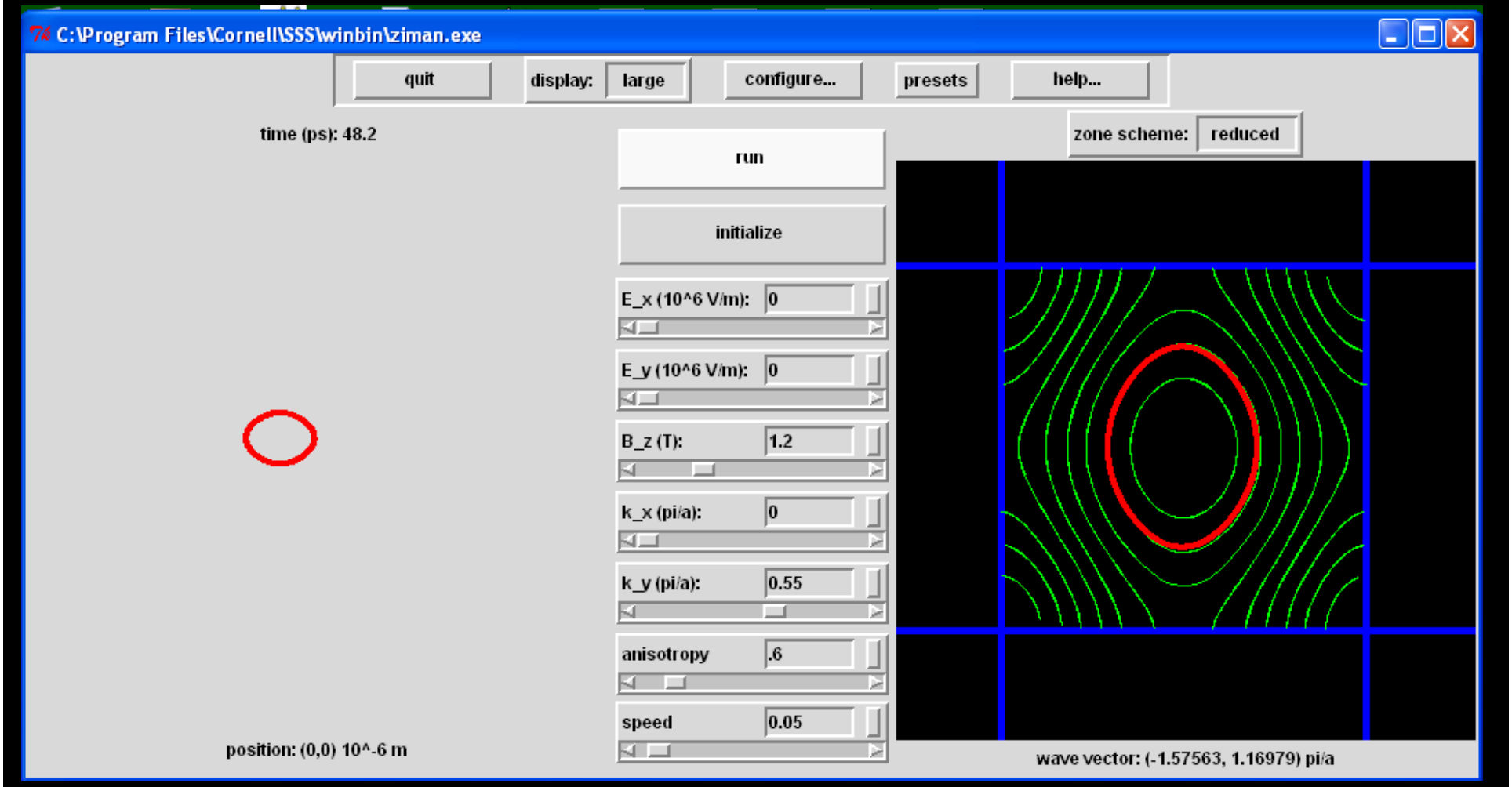
$$\vec{b}_1 = \frac{2\pi}{a}\,\hat{k_x} - \frac{2\pi\cos\gamma}{a\sin\gamma}\,\hat{k_y}, \qquad \vec{b}_2 = \frac{2\pi}{b\sin\gamma}\,\hat{k_y}.$$

$$G_{hk,x} = hb_{1,x} + kb_{2,x} \text{ and } G_{hk,y} = hb_{1,y} + kb_{2,y}.$$

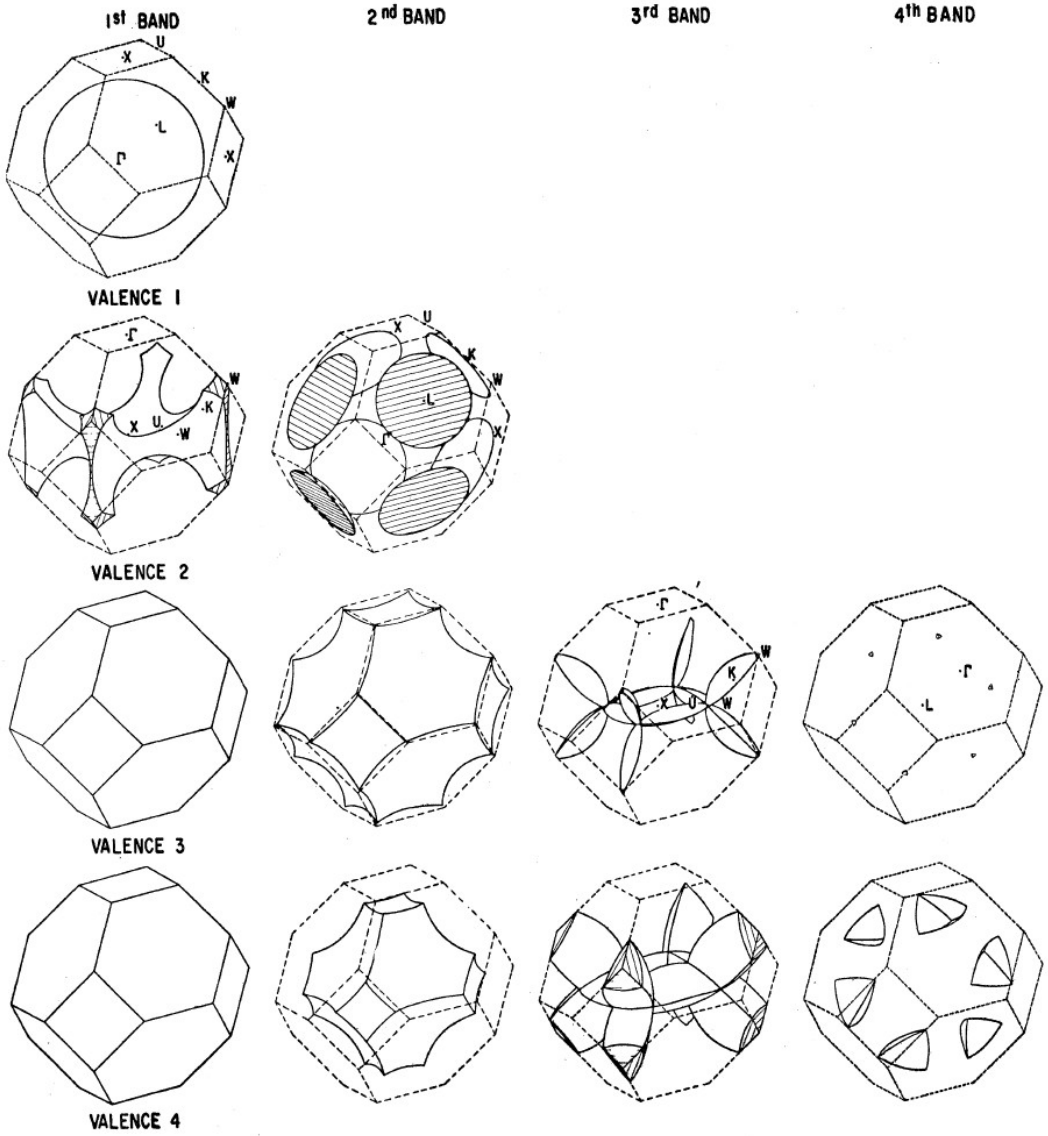
$$G_{hk,x}k_x + G_{hk,y}k_y = \frac{G_{hk,x}^2}{2} + \frac{G_{hk,y}^2}{2},$$



http://lampx.tugraz.at/~hadley/ss2/fermisurface/2d_fermisurface/2dBz.php

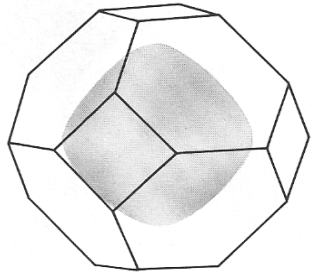

C:\Program Files\Cornell\SSS\winbin\ziman.exe
quit
display:
large
configure...
presets
help...
time (ps): 48.2
run
initialize
zone scheme:
reduced
E_x (10^6 V/m):
0
E_y (10^6 V/m):
0
B_z (T):
1.2
k_x (pi/a):
0
k_y (pi/a):
0.55
anisotropy
.6
speed
0.05
position: (0,0) 10^-6 m
wave vector: (-1.57563, 1.16979)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

Fermi surface for fcc in the empty lattice approximation

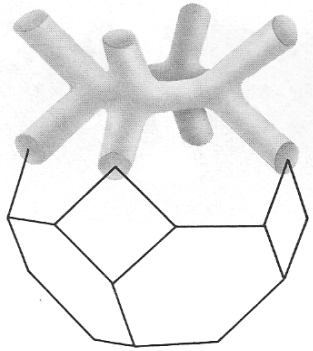


Valence 4

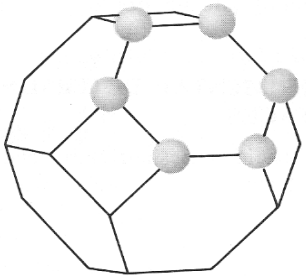
2nd zone holes



3rd zone monster



4th zone electrons



Fermi Surfaces

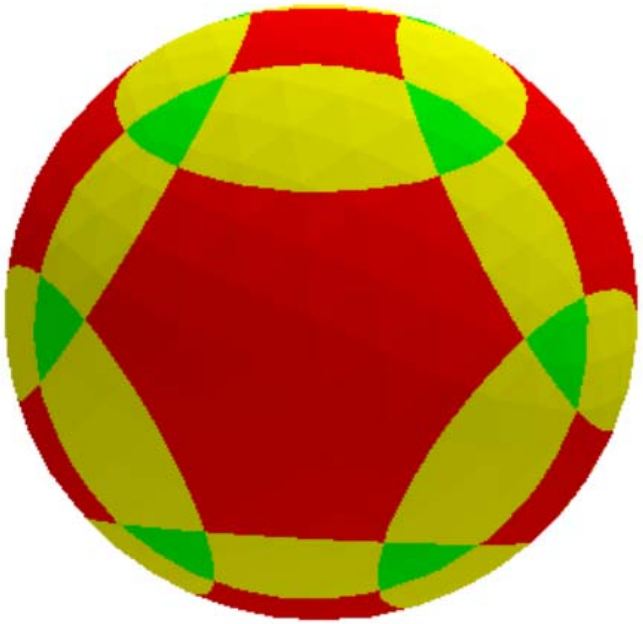
n =3.6 [-] [+] electrons/unit cell

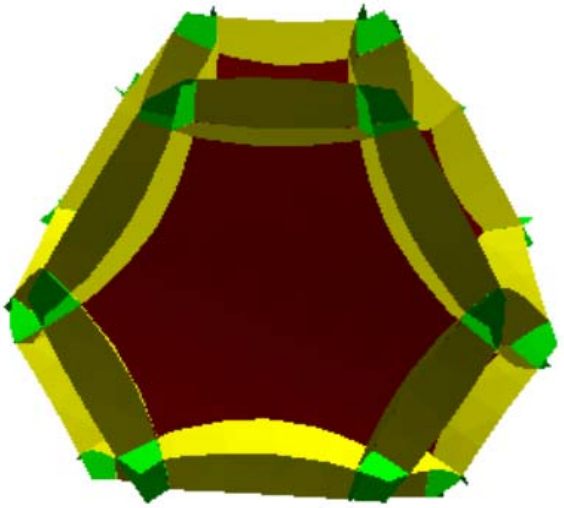
$$k_F = (3\pi^2 n)^{1/3} = 4.74$$

Lattice: ○ Simple Cubic ○ Body Centered Cubic ◉ Face Centered Cubic ○ Hexagonal Close Pack $\frac{c}{a} = \sqrt{\frac{8}{3}}$

[Show 1st Brillouin zone] [Stop Rotation]

Brillouinzone	1	2	3	4
Outside Color				
Inside Color				
Show	☑	☑	☑	☑





http://lampx.tugraz.at/~hadley/ss2/fermisurface/3d_fermisurface/index.html