3. Electrons

Oct 8, 2018

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}

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:

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

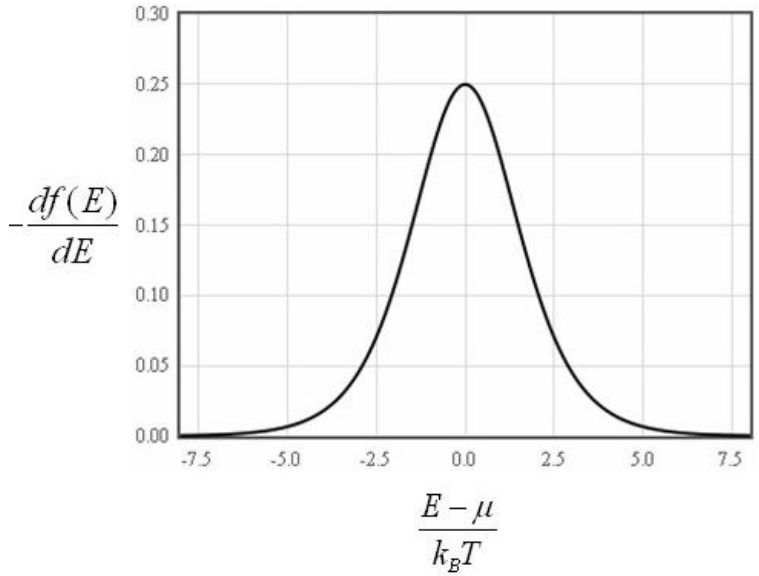
DoS → cv(T)

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

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

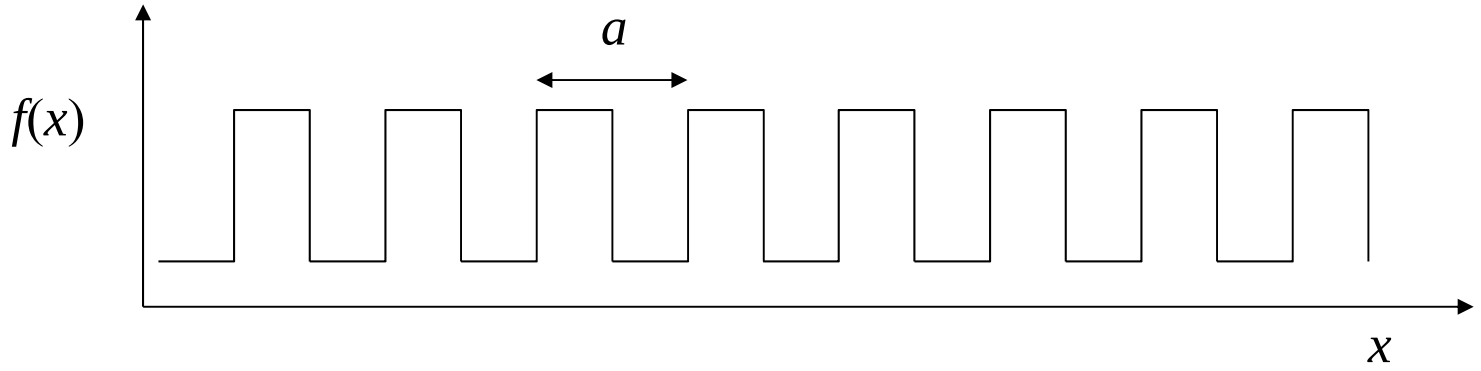
$$n = \int_{-\infty}^{\infty} D(E) f(E) dE = \int_{-\infty}^{\infty} \frac{D(E) dE}{\exp\left(\frac{E-\mu}{k_B T}\right)+1}.$$

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



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

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

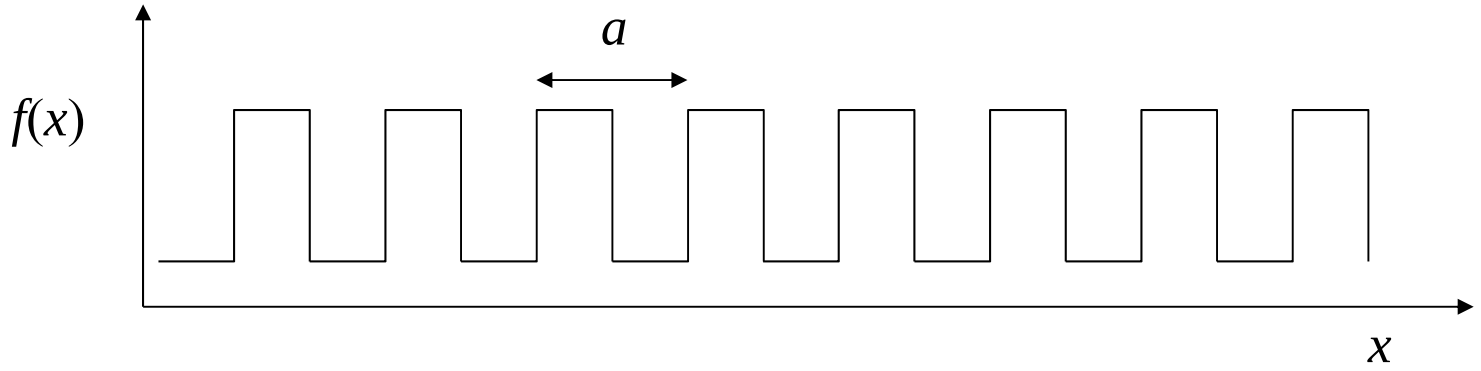
$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

multiply by $\cos(2\pi p'x/a)$ and integrate over a period.

$$\int_0^a f(x)\cos\left(2\pi px/a\right)dx = c_p \int_0^a \cos\left(2\pi px/a\right)\cos\left(2\pi px/a\right)dx = \frac{ac_p}{2}$$

$$c_p = \frac{2}{a}\int_0^a f(x)\cos\left(2\pi px/a\right)dx$$

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \qquad \sin x = \frac{e^{ix} - e^{-ix}}{2i}$$

$$f(x) = \sum_{G=-\infty}^{\infty} f_G e^{iGx} \qquad f_G = \frac{c_p}{2} - i\frac{s_p}{2} \qquad G = \frac{2\pi p}{a}$$

For real functions: $f_G^* = f_{-G}$

reciprocal lattice vector

Fourier series in 1-D, 2-D, or 3-D

In two or three dimensions, a periodic function can be thought of as a pattern repeated on a Bravais lattice. It can be written as a Fourier series

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Reciprocal lattice vectors
(depend on the Bravais lattice)

Structure factors
(complex numbers)

In 1-D:

$$\vec{G} = v\vec{b} \qquad v = -\infty \ldots -1, 0, 1, \ldots \infty \qquad \left|\vec{b}\right| = \frac{2\pi}{a}$$

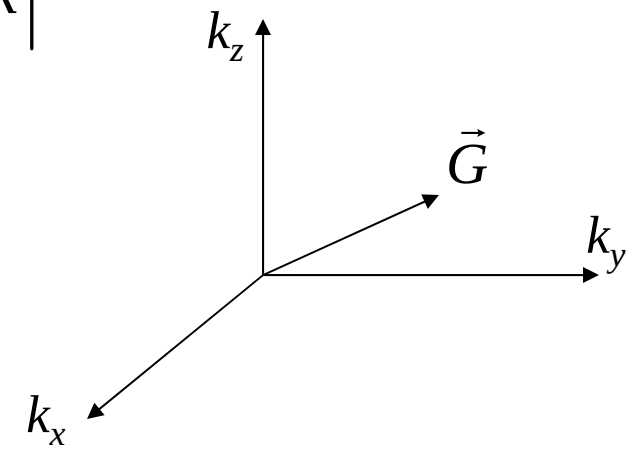
Reciprocal space (Reziproker Raum)
k-space (*k*-Raum)

k-space is the space of all wave-vectors.

A *k*-vector points in the direction a wave is propagating.

wavelength: $\lambda = \frac{2\pi}{|\vec{k}|}$

momentum: $\vec{p} = \hbar\vec{k}$



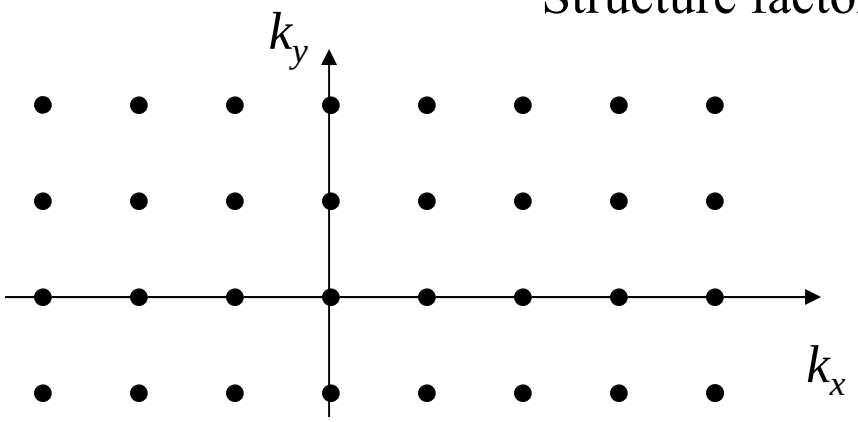
Reciprocal lattice (Reziprokes Gitter)

Any periodic function can be written as a Fourier series

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Reciprocal lattice vector G

Structure factor



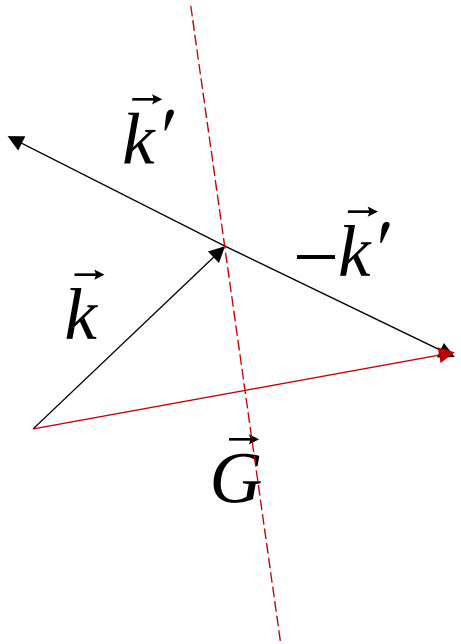
$$\vec{G} = \upsilon_1\vec{b}_1 + \upsilon_2\vec{b}_2 + \upsilon_3\vec{b}_3$$

ν_i integers

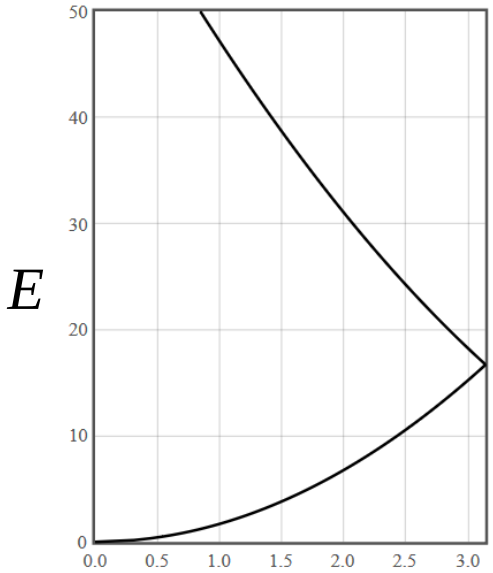
$$\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}, \qquad \vec{b}_2 = 2\pi\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}, \qquad \vec{b}_3 = 2\pi\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}$$

Diffraction condition

$$\Delta\vec{k} = \vec{G}$$

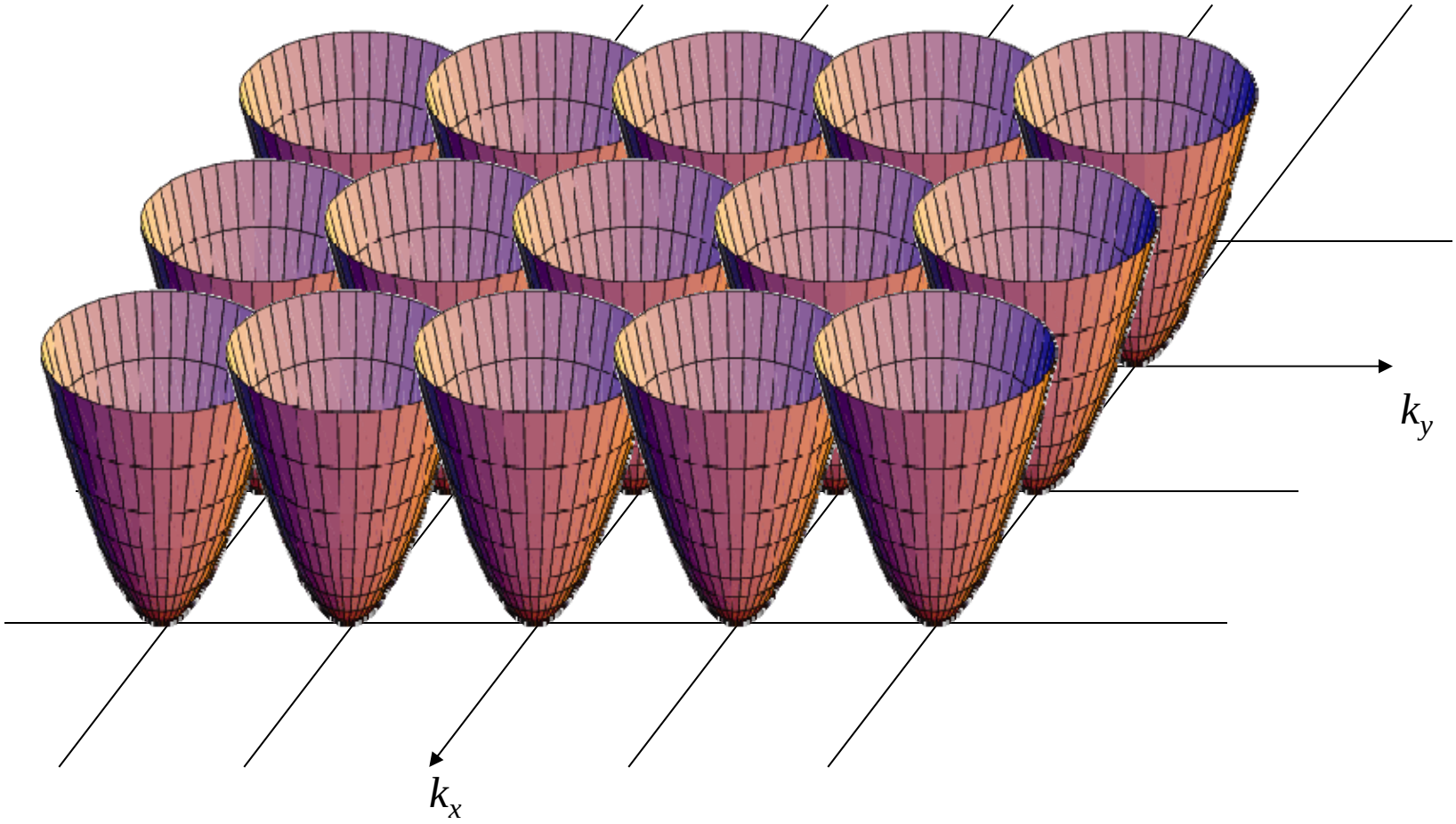


Empty lattice approximation



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

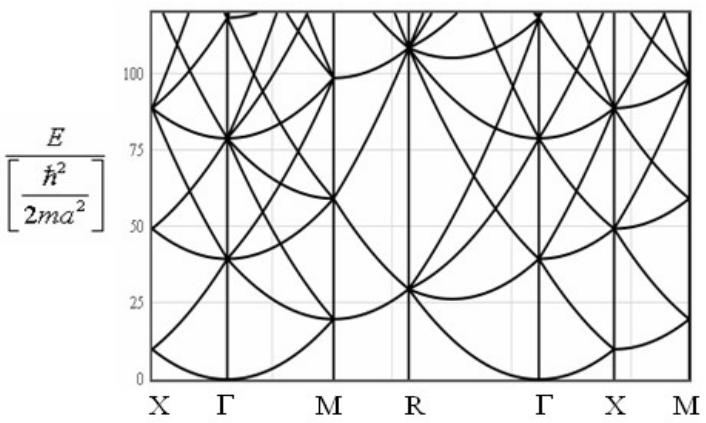
Empty lattice approximation



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

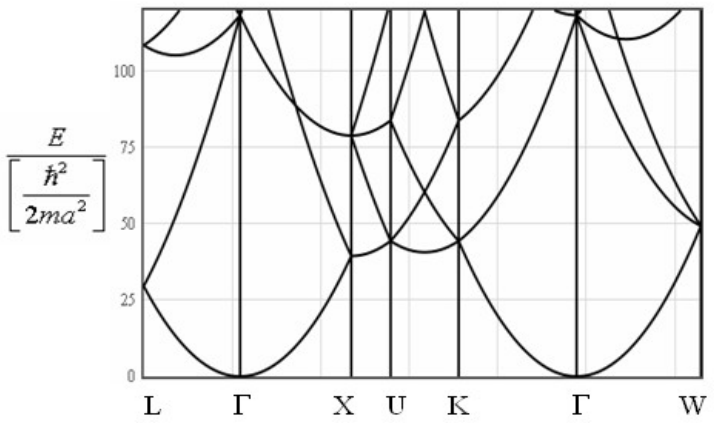
Empty lattice approximation

Simple cubic



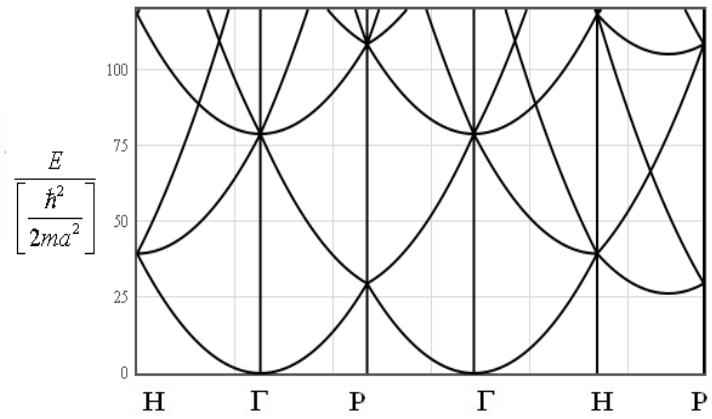
Choose a different order for the symmetry points

Face centered cubic

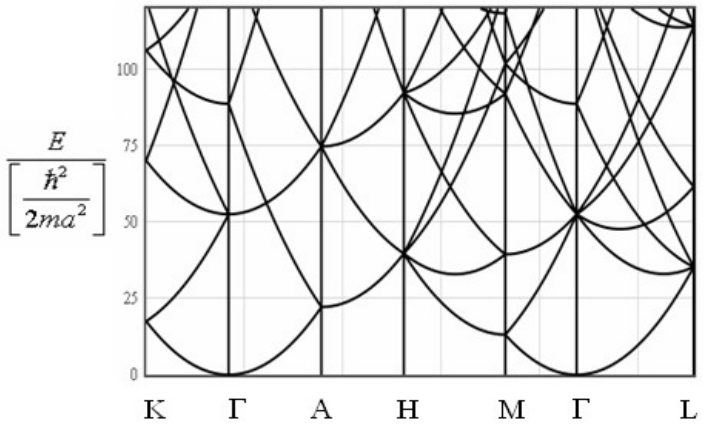


Choose a different order for the symmetry points

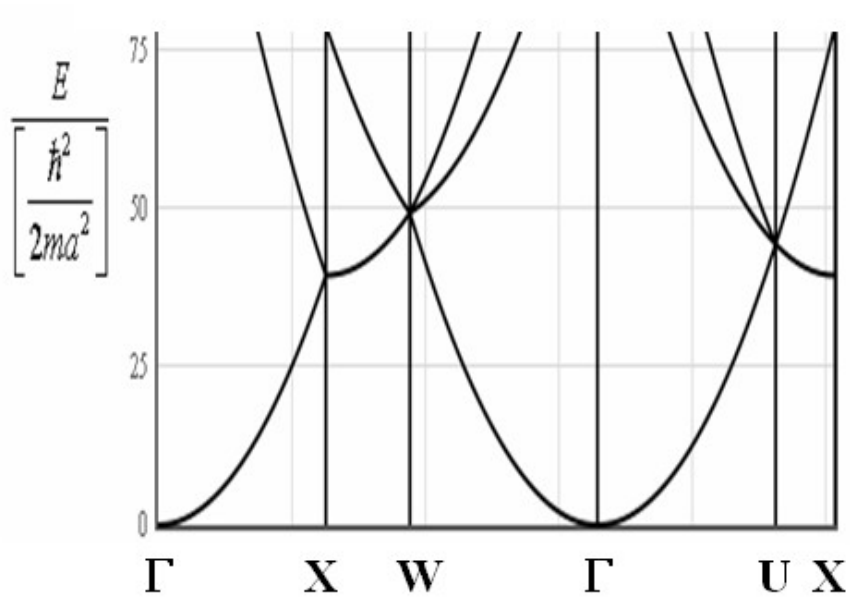
Body centered cubic

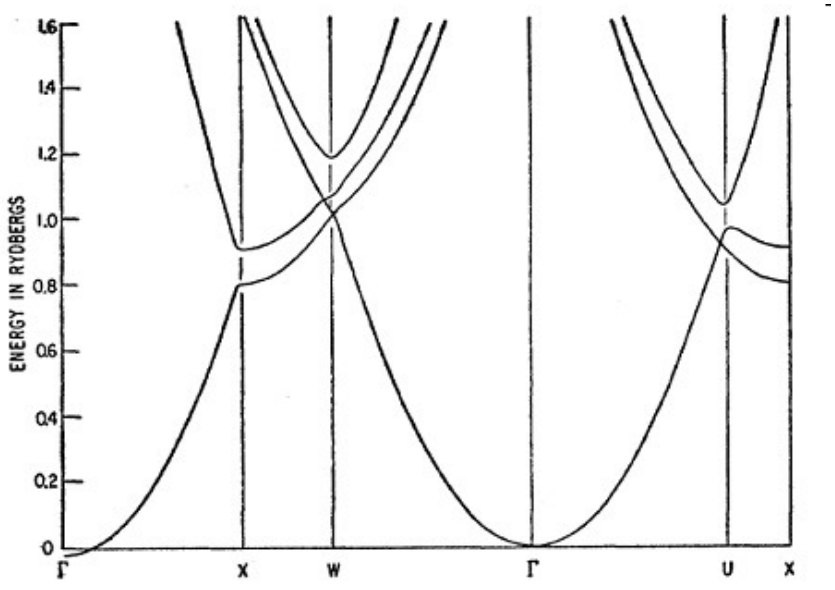


Hexagonal



Empty lattice approximation

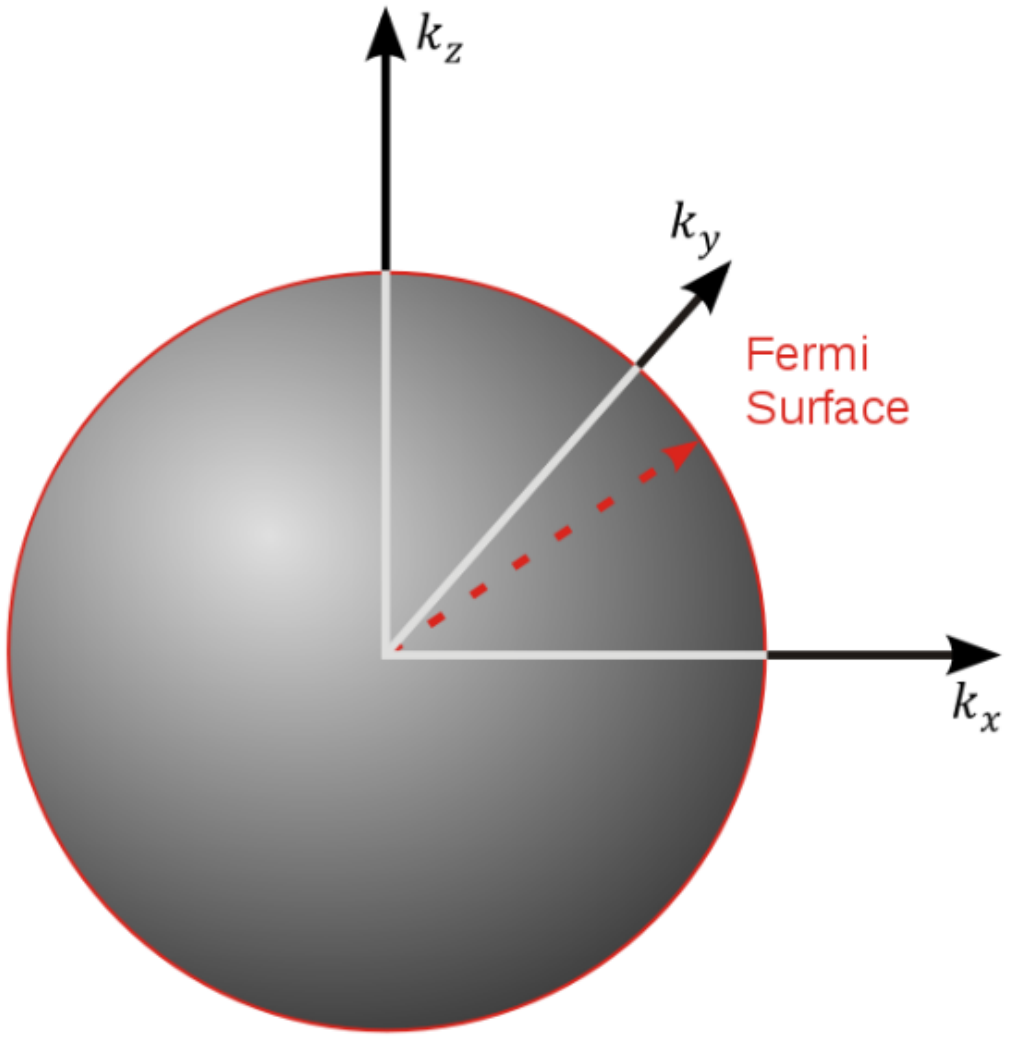




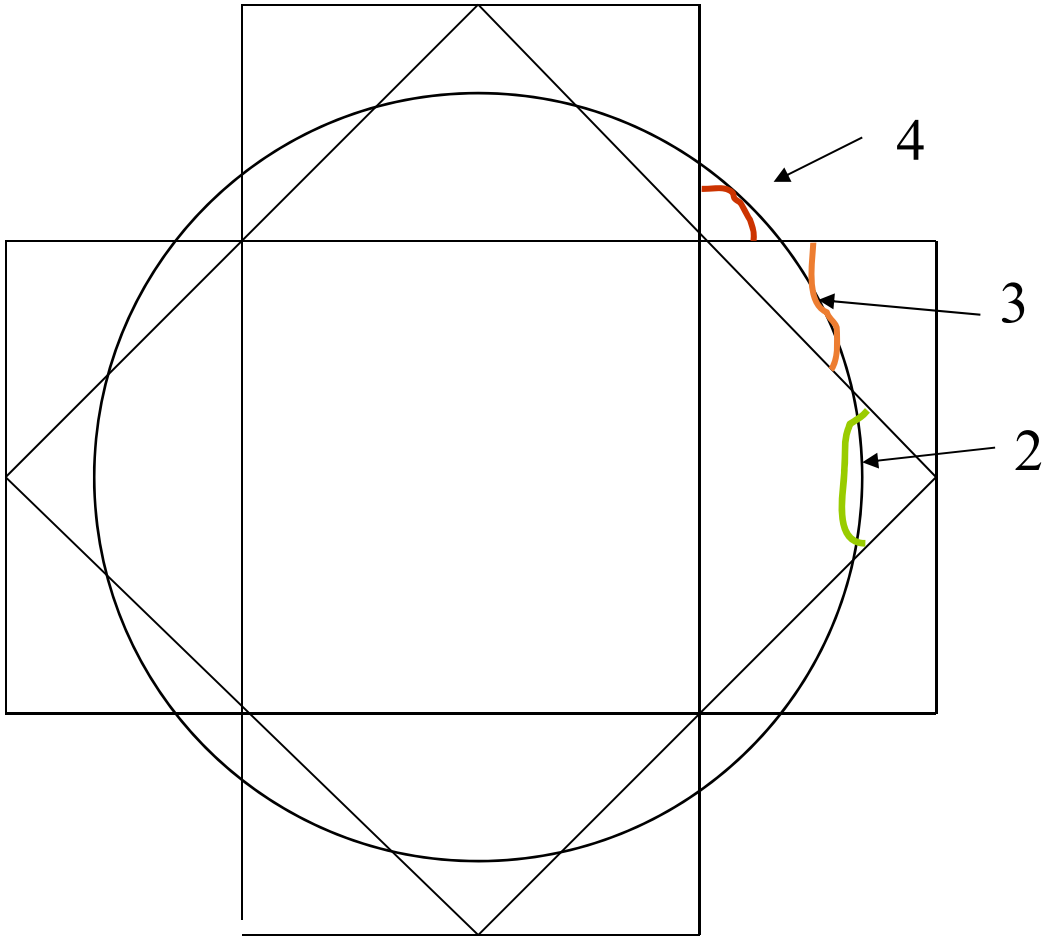
W. Harrison, Phys. Rev. 118 p. 1182 (1960)

aluminum

Fermi surface for free electrons



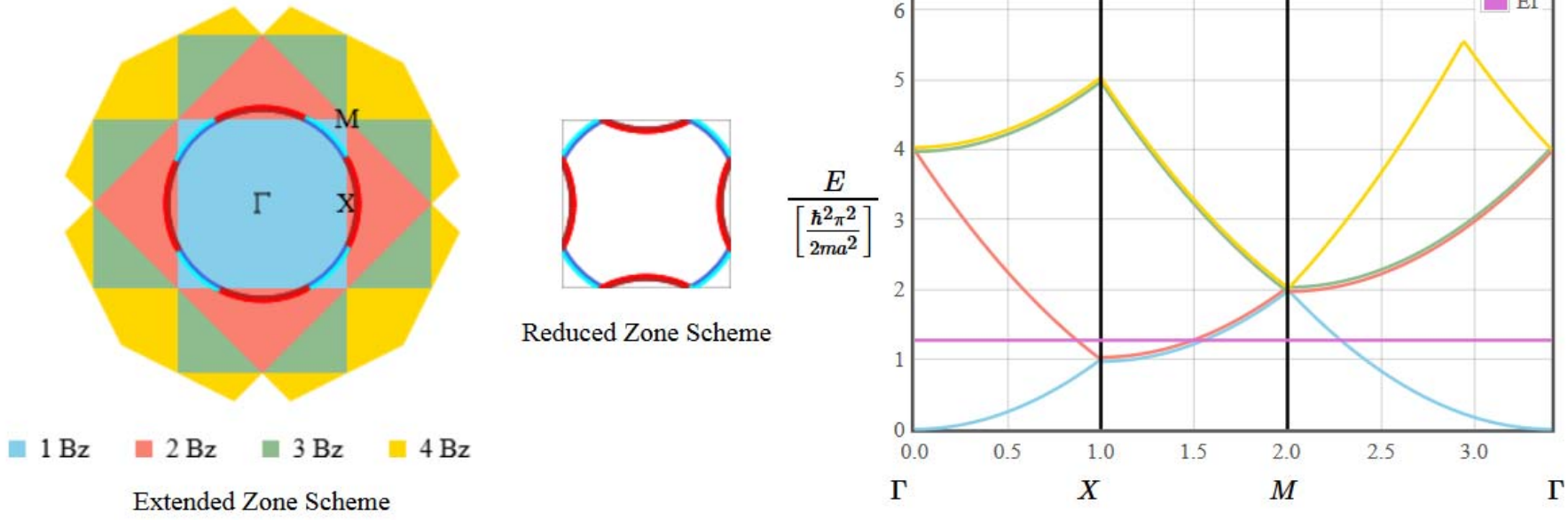
Constructing Fermi surface



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

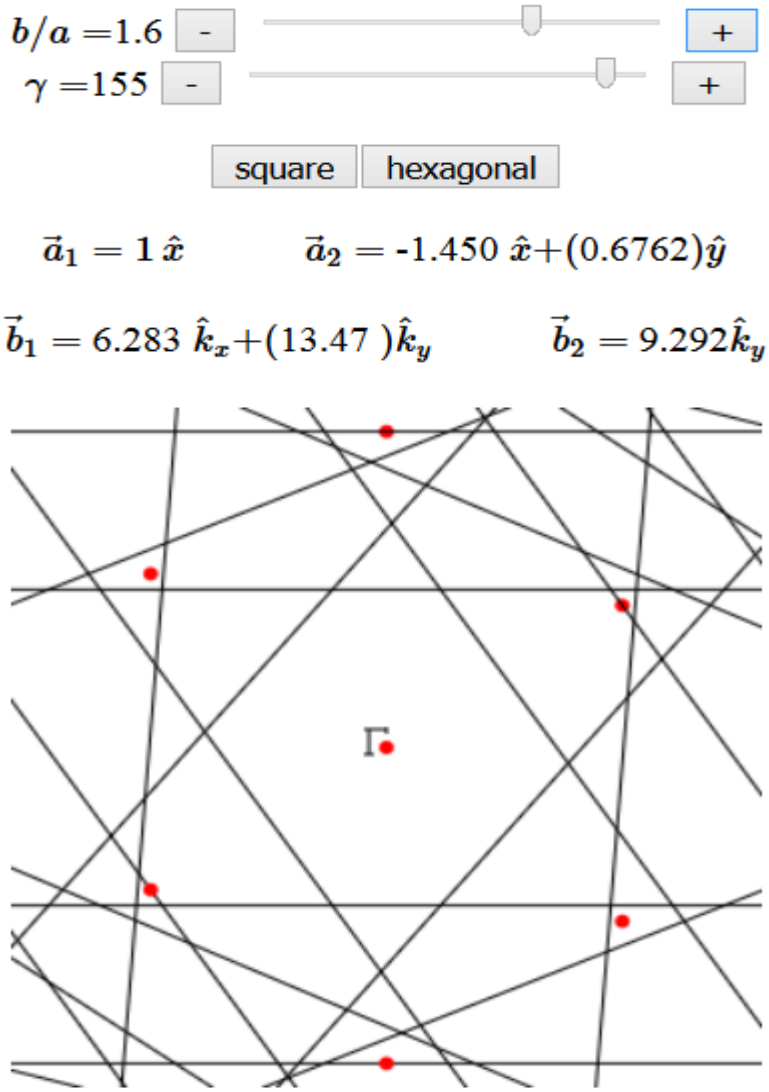
$$\vec{a}_1 = a\,\hat{x}, \qquad \vec{a}_2 = b\cos\gamma\,\hat{x} + b\sin\gamma\,\hat{y}.$$

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

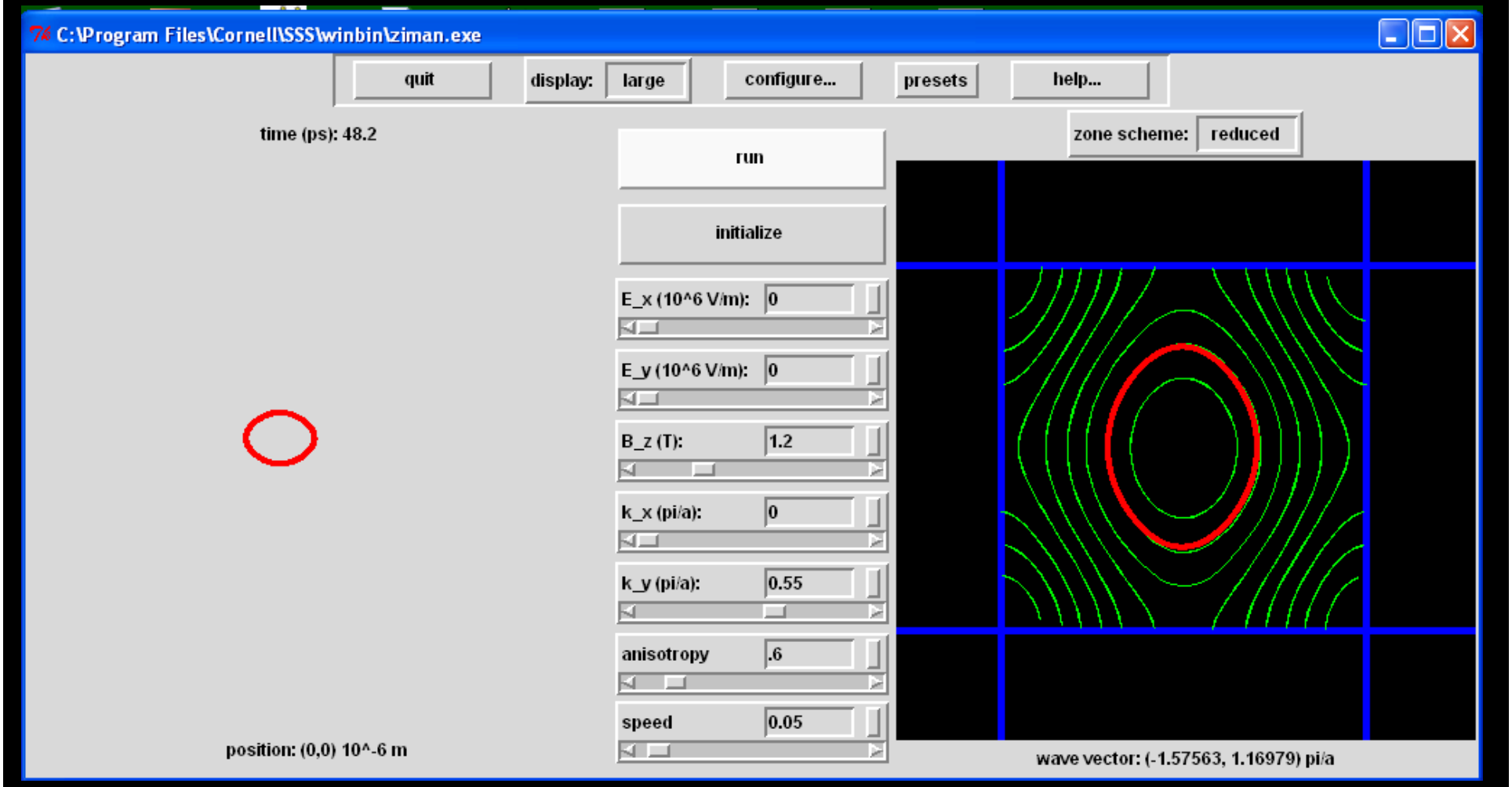
$$\vec{b}_1 = \frac{2\pi}{a}\,\hat{k_x} - \frac{2\pi\cos\gamma}{a\sin\gamma}\,\hat{k_y}, \qquad \vec{b}_2 = \frac{2\pi}{b\sin\gamma}\,\hat{k_y}.$$

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

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



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