Fourier Transforms

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

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

Reciprocal lattice vectors G
(depend on the Bravais lattice)

Structure factors
(complex numbers)

$$\vec{T}_{hkl} = h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} \qquad \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0, & \text{for } i \neq j \end{cases}$$

$$\vec{G} = \nu_1\vec{b}_1 + \nu_2\vec{b}_2 + \nu_3\vec{b}_3$$

Fourier transforms

Most functions can be expressed in terms of plane waves

$$f(\vec{r}) = \int F\left(\vec{k}\right) e^{i\vec{k}\cdot\vec{r}}\, d\vec{k}$$

This can be inverted for $F(k)$

$$F\left(\vec{k}\right) = \frac{1}{(2\pi)^d} \int f(\vec{r}) e^{-i\vec{k}\cdot\vec{r}}\, d\vec{r}$$

Fourier transform of $f(r)$

http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/ft/ft.php

$\exp(-\lvert a\rvert x)$	$\frac{\lvert a\rvert}{\pi(a^2+k^2)}$	$\frac{2\lvert a\rvert}{a^2+k^2}$
$\operatorname{sgn}(x)$ $\operatorname{sgn}(x) = -1$ for $x < 0$ and $\operatorname{sgn}(x) = 1$ for $x > 0$	$\frac{-i}{\pi\omega}$	$\frac{-2i}{\omega}$
$\operatorname{sgn}(x)\exp(-\lvert a\rvert x)$	$\frac{-ik}{\pi(a^2+k^2)}$	$\frac{-i2k}{a^2+k^2}$
$H(x)\exp(-\lvert a\rvert x)$	$\frac{\lvert a\rvert-ik}{2\pi(a^2+k^2)}$	$\frac{\lvert a\rvert-ik}{a^2+k^2}$
$\sqcap(x) = H\left(x+\frac{1}{2}\right)H\left(\frac{1}{2}-x\right)$ Square pulse: height = 1, width = 1, centered at $x = 0$.	$\frac{\sin(k/2)}{\pi k}$	$\frac{2\sin(k/2)}{k}$
$\sqcap\left(\frac{x-x_0}{a}\right)$ Square pulse: height = 1, width = a, centered at x_0.	$\frac{\sin(ka/2)}{\pi k}\exp(-ikx_0)$	$\frac{2\sin(ka/2)}{k}\exp(-ikx_0)$
$\exp\left(i\vec{k}_0\cdot\vec{r}\right)$ Plane wave	$\delta\left(\vec{k}-\vec{k}_0\right)$	$(2\pi)^d\delta\left(\vec{k}-\vec{k}_0\right)$
1	$\delta(k)$	$2\pi\delta(k)$
$\delta(x)$	$\frac{1}{2\pi}$	1
$\delta\left(\frac{\vec{r}-\vec{r}_0}{a}\right)$	$\left(\frac{a}{2\pi}\right)^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$a^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$\exp\left(-\frac{\lvert\vec{r}-\vec{r}_0\rvert^2}{a^2}\right)$	$\left(\frac{a}{2\sqrt{\pi}}\right)^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$\left(a\sqrt{\pi}\right)^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$H(R-\lvert\vec{r}-\vec{r}_0\rvert)$ Disc of radius R centered at $\vec{r}_0$, $\vec{r}\in\mathrm{R}^2$	$\frac{R}{2\pi\lvert\vec{k}\rvert}J_1(\lvert\vec{k}\rvert R)\exp(-i\vec{k}\cdot\vec{r}_0)$	$\frac{2\pi R}{\lvert\vec{k}\rvert}J_1(\lvert\vec{k}\rvert R)\exp(-i\vec{k}\cdot\vec{r}_0)$
$H(R-\lvert\vec{r}-\vec{r}_0\rvert)$ Sphere of radius R centered at $\vec{r}_0$, $\vec{r}\in\mathrm{R}^3$	$\frac{1}{(2\pi)^3\lvert\vec{k}\rvert^3}\left(\sin(\lvert\vec{k}\rvert R)-\lvert\vec{k}\rvert R\cos(\lvert\vec{k}\rvert R)\right)\exp(-i\vec{k}\cdot\vec{r}_0)$	$\frac{4\pi}{\lvert\vec{k}\rvert^3}\left(\sin(\lvert\vec{k}\rvert R)-\lvert\vec{k}\rvert R\cos(\lvert\vec{k}\rvert R)\right)\exp(-i\vec{k}\cdot$

Here $H(x)$ is the Heaviside step function, $\delta(x)$ is the Dirac delta function, $J_1(x)$ is the first order Bessel function of the first kind, and d is the number of dimensio

Calculate a Fourier transform numerically.

http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/ft/ft.php

Fourier transforms

The Fourier transform of a function $f(t)$ using the [1,-1] notation is,

$$\mathcal{F}(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt.$$

Consider a function that is nonzero only in the interval $t_1 < t < t_2$. The Fourier transform in this case is,

$$\mathcal{F}(\omega) = \int_{t_1}^{t_2} f(t) e^{-i\omega t} dt.$$

The following form can be used to define $f(t)$ between t_1 and t_2. The function $f(t)$ as well as its Fourier transform $\mathcal{F}(\omega)$ are tabulated and plotted.

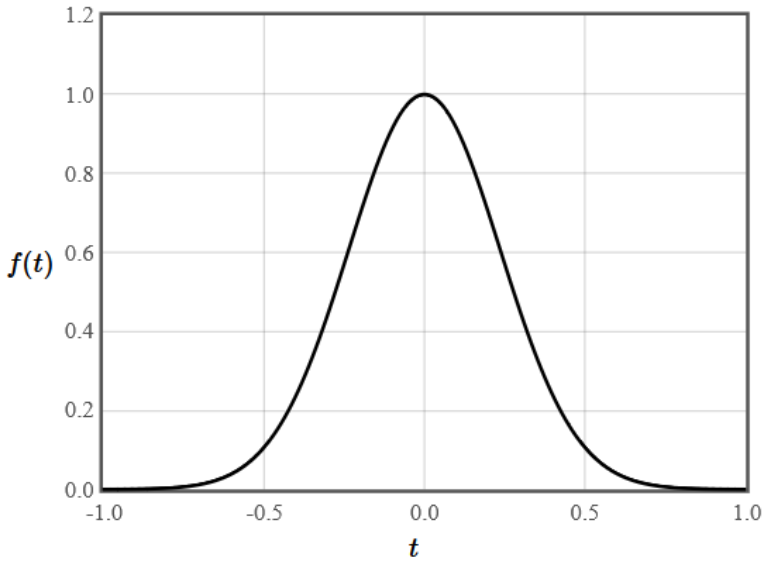
$f(t) =$ exp(-9*t*t) ?+ ?-

Calculate Fourier Transform where $t_1 =$ -1 and $t_2 =$ 1 for frequencies $|\omega| <$ 24.

sine | cosine | Gaussian | Gaussian derivative | square | shifted square | triangle | beats | even pulse | odd pulse | exp(-|t|/τ) | sgn(t)exp(-|t|/τ) | H(t)exp(-t/τ) | H(t)exp(-

The Fourier transform of a Gaussion is a Gaussian. Since the Gaussian is an even function, the Fourier transform is real.

t	$f(t)$
-1	0.00012340980408667956
-0.998	0.00012792888893978386
-0.996	0.00013260390913379999
-0.994	0.00013743987626671717
-0.992	0.00014244195137793746
-0.99	0.00014761544652796337
-0.988	0.00015296582921188573
-0.986	0.00015849872640165 66
-0.984	0.00016421992867658 14
-0.982	0.00017013539444340507
-0.98	0.00017625125424738458



Fourier analysis of real data sets

Consider a series of N measurements x_n that are made at equally spaced time intervals Δt. The total time to make the measurement series is $N\Delta t$. A discrete Fourier transform can be used to find a periodic function $x(t)$ with a fundamental period $N\Delta t$ that passes through all of the points. This function can be expressed as a Fourier series in terms of sines and cosines,

$$x(t) = \sum_{n=0}^{n<N/2} \left[a_n \cos\left(\frac{2\pi nt}{N\Delta t}\right) + b_n \sin\left(\frac{2\pi nt}{N\Delta t}\right) \right]. \tag{1}$$

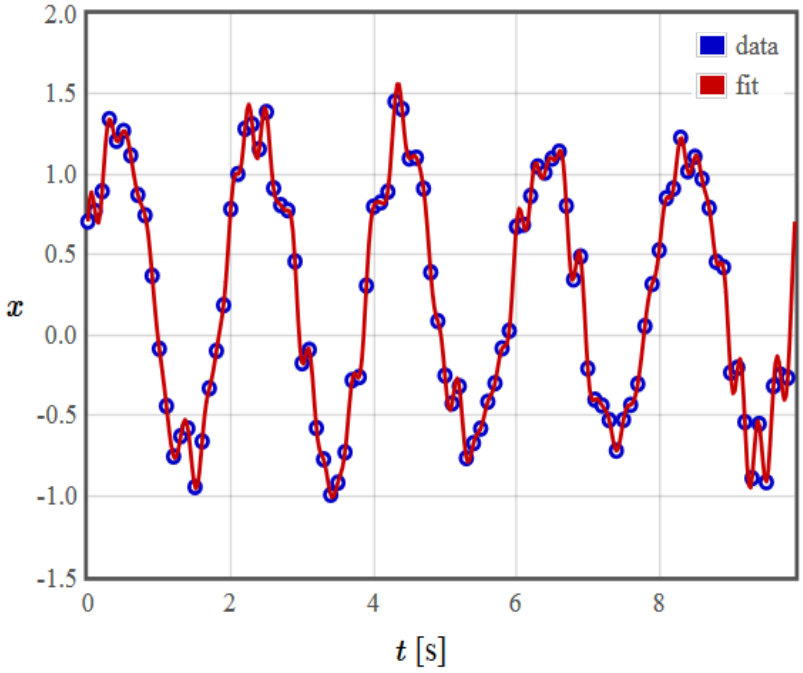
Data for x_n can be input in the textbox below. When the 'Calculate Fourier Coefficients' button is pressed, the periodic function $x(t)$ is plotted through the data points. The Fourier coefficients are tabulated and plotted as well. The fft algorithm first checks if the number of data points is a power-of-two. If so, it calculates the discrete Fourier transform using a Cooley-Tukey decimation-in-time radix-2 algorithm. If the number of data points is not a power-of-two, it uses Bluestein's chirp z-transform algorithm. The fft code was taken from Project Nayuki.

x_n

```
0.704755992151468
0.7702905111005827
0.8931618373710344
1.3406823044010674
1.2059826464418861
1.2675358230469096
1.1156175628382647
0.8703050439010842
0.7442227455673327
0.3681609224807739
-0.08539320011647894
```

$\Delta t =$ 0.1 s

Calculate Fourier Coefficients

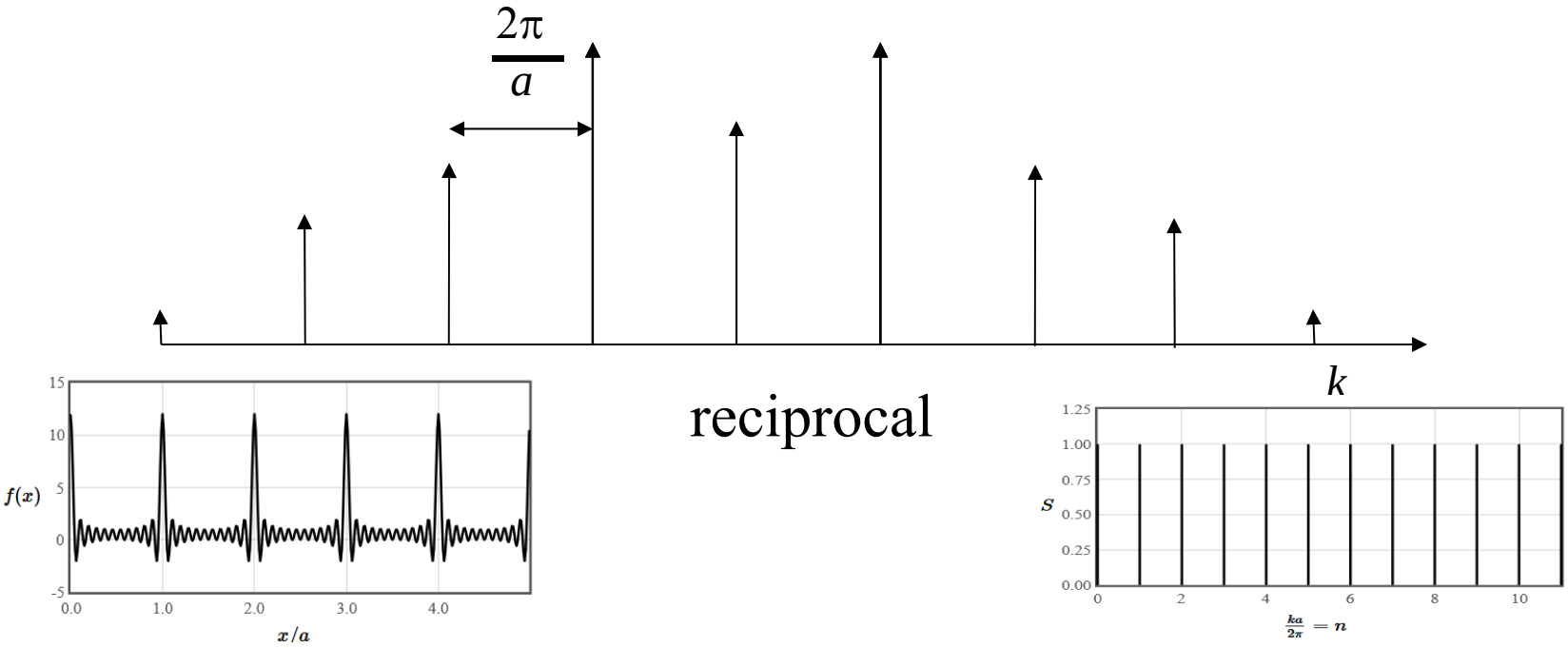


http://lampx.tugraz.at/~hadley/num/ch3/3.3a.php

The reciprocal lattice is the Fourier transform of the real space lattice

$$\text{crystal} = \text{Bravais\_lattice}(r) * \text{unit\_cell}(r)$$

$$\mathcal{F}(\text{crystal}) = \mathcal{F}(\text{Bravais\_lattice}(r))\mathcal{F}(\text{unit\_cell}(r))$$



Free electron Fermi gas

Kittel, chapter 6

Gross and Marx: Das freie Elektronengas 7.1-7.2

A simple model for a metal is electrons confined to box with periodic boundary conditions.

Band structure calculations

Start with the full Hamiltonian.

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A}\nabla_A^2 - \sum_{i,A} \frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j} \frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{A<B} \frac{Z_A Z_B e^2}{4\pi\varepsilon_0 r_{AB}}$$

Everything you can know is contained in this Hamiltonian.

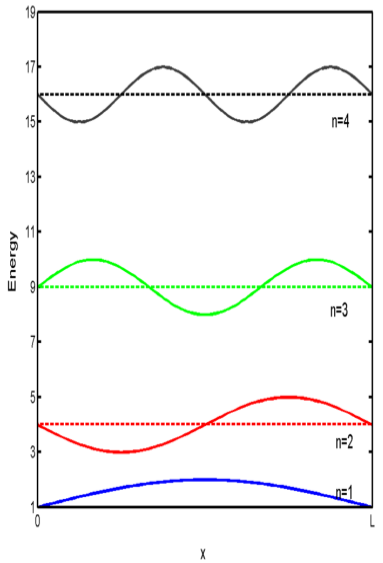
Usually this is too difficult to solve.

http://en.wikipedia.org/wiki/File:Erwin_Schr%C3%B6dinger.jpg

Free particles in 1-d

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad V = 0$$

$$E = \frac{mv^2}{2} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{n^2 h^2}{8mL^2}$$



$$\lambda = \frac{2L}{n}$$

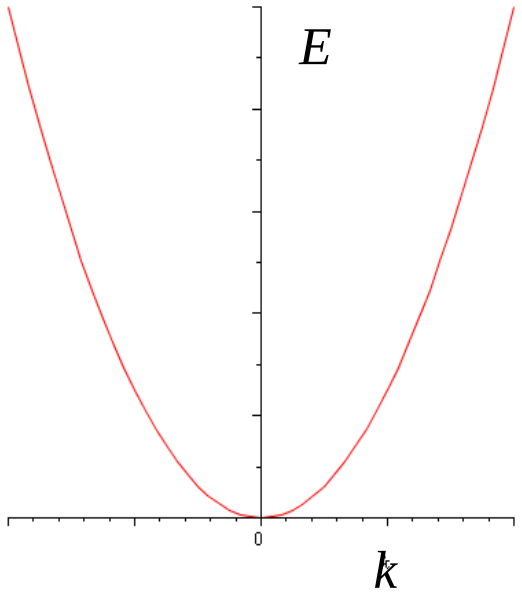
Free particles

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \qquad V = 0$$

plane wave

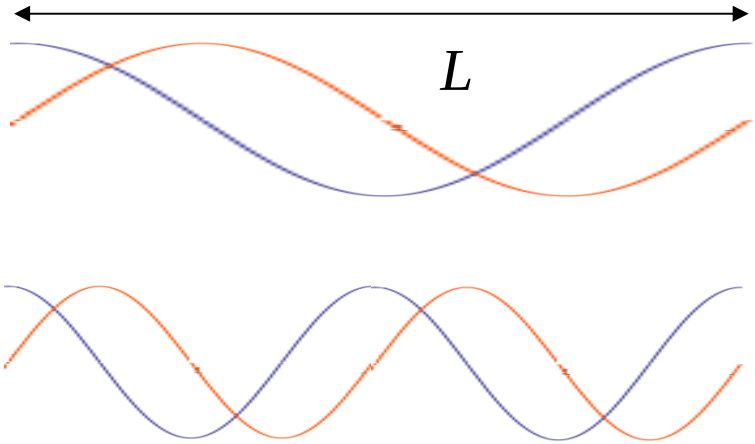
Eigen function solutions: $\psi_k = A_k e^{i(kx-\omega t)}$

Dispersion relation: $E = \hbar\omega = \frac{\hbar^2 k^2}{2m} = \frac{1}{2}mv^2$



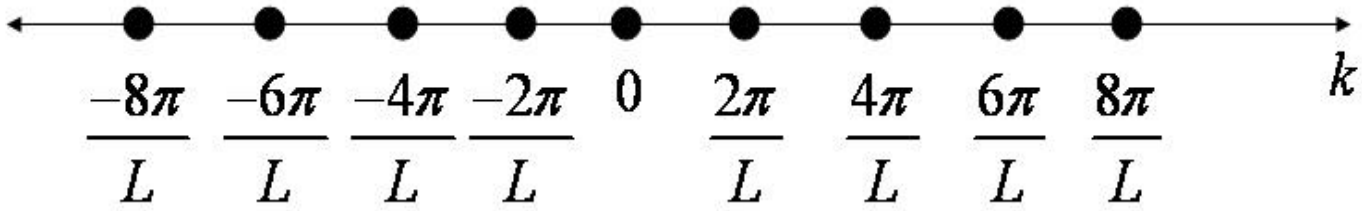
Periodic boundary conditions

$$\psi = A_k e^{i(kx-\omega t)}$$



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

$$\frac{4\pi}{L}$$



$$LD(k)dk = \frac{2 \cdot 2dk}{\frac{2\pi}{L}}$$

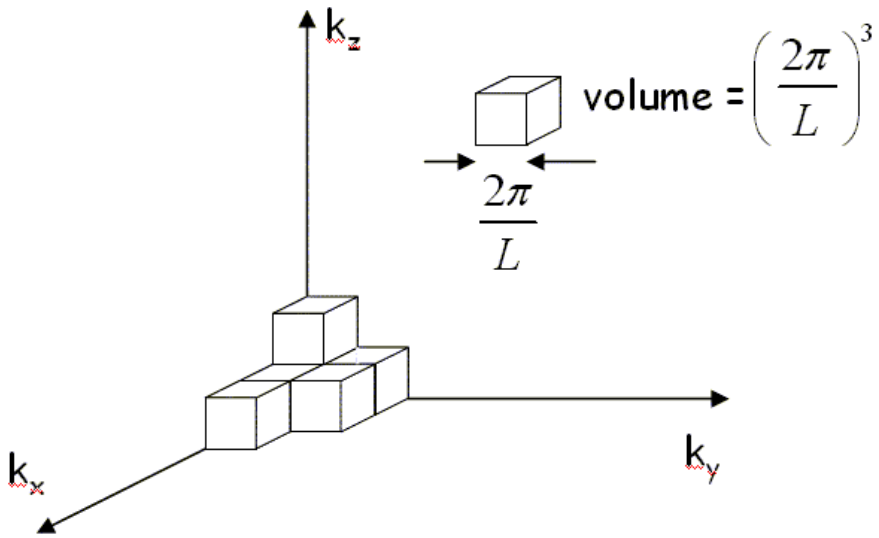
Density of states:

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

← Spin

Number of states between $|k|$ and $|k|+dk$ is $LD(k)dk$

Density of states



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

Number of states between k and $k+dk$ for a box of size L^3.

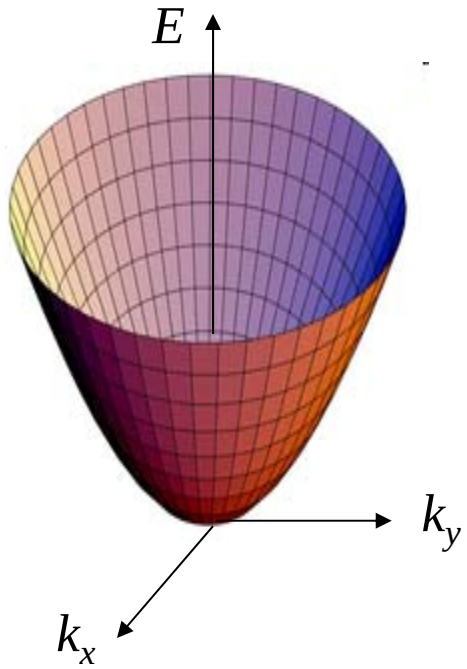
$$= 2\frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3} = \frac{k^2 L^3}{\pi^2} dk = L^3 D(k) dk$$

spin

$D(k) = k^2/\pi^2$ = density of states/m^3

Free particles in 3-d

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



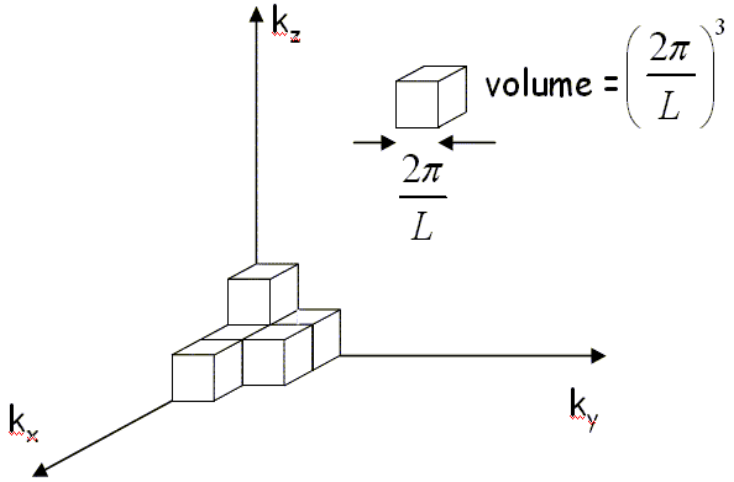
Density of states

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

$$k^2 = \frac{2mE}{\hbar^2}$$

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

$$D(E) = D(k)\frac{dk}{dE}$$



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

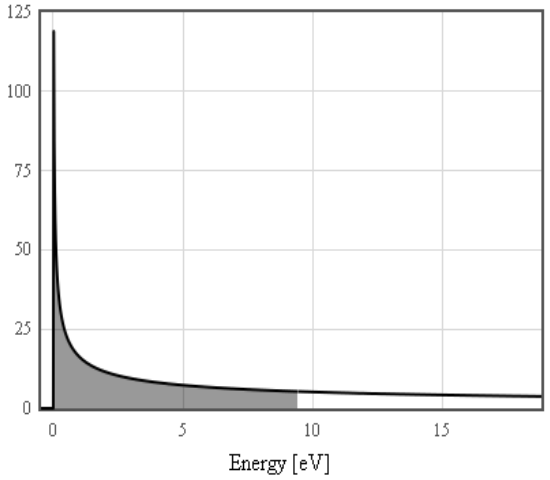
$$\boxed{D(E) = \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E}}$$

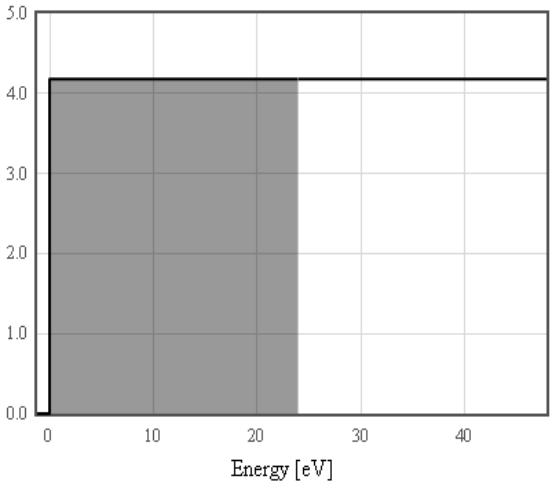
Free electron Fermi gas

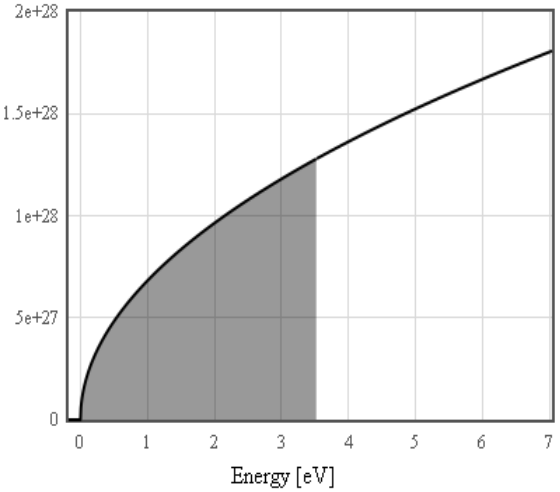
1 - d $$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \quad \mathrm{J^{-1}m^{-1}}$$

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

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



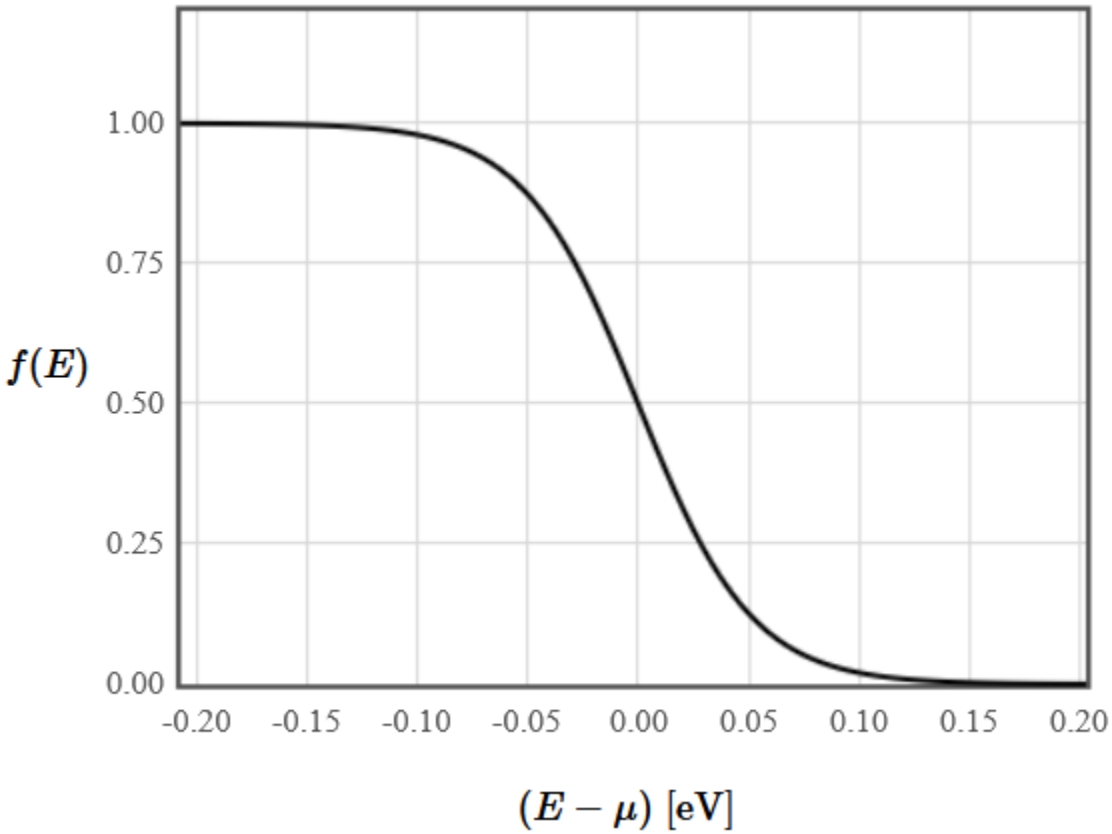


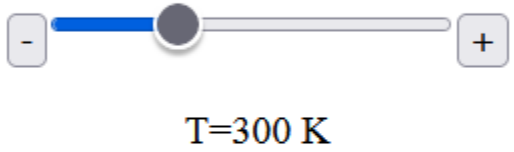


Fermi function

$f(E)$ is the probability that a state at energy E is occupied.

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





μ = chemical potential

Fermi energy

In solid state physics books,

$$E_F = \mu(T=0).$$

In semiconductor books, $E_F(T) = \mu(T)$.

$$\text{At } T = 0 \qquad n = \int_{-\infty}^{E_F} D(E)dE$$

In three dimensions,

$$n = \frac{N}{L^3} = \frac{\sqrt{2}m^{3/2}}{\pi^2\hbar^3}\int_0^{E_F}\sqrt{E}dE = \frac{(2m)^{3/2}}{3\pi^2\hbar^3}E_F^{3/2}$$

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

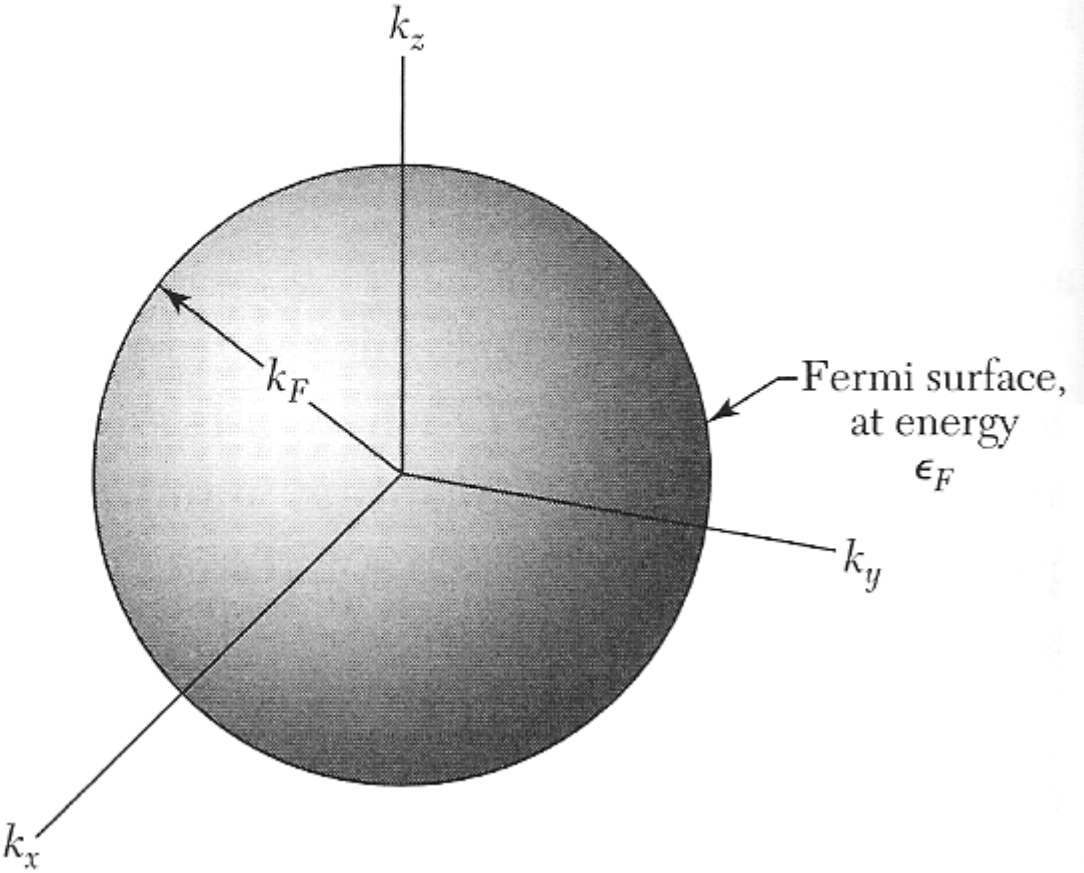
Fermi sphere

$$N = 2\frac{4\pi k_F^3}{3\left(\frac{2\pi}{L}\right)^3}$$

spin

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

n = electron density



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

The thermal and electronic properties depend on the states at the Fermi surface.

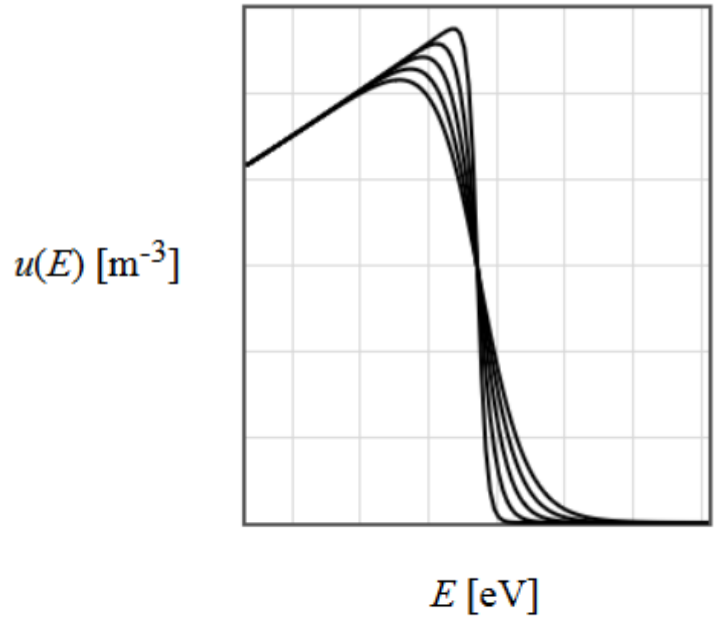
Free particles in 1-d

internal energy spectral density

$$u(E) = ED(E)f(E) = \frac{\pi}{2}\left(\frac{2m}{\hbar^2\pi^2}\right)^{3/2} \frac{1}{\exp\left(\frac{E-\mu}{k_B T}\right)+1} E^{\frac{3}{2}}$$

$$u = \int_{-\infty}^{\infty} u(E)dE$$

$$c_v = \frac{du}{dT}$$



Not possible to do this integral analytically

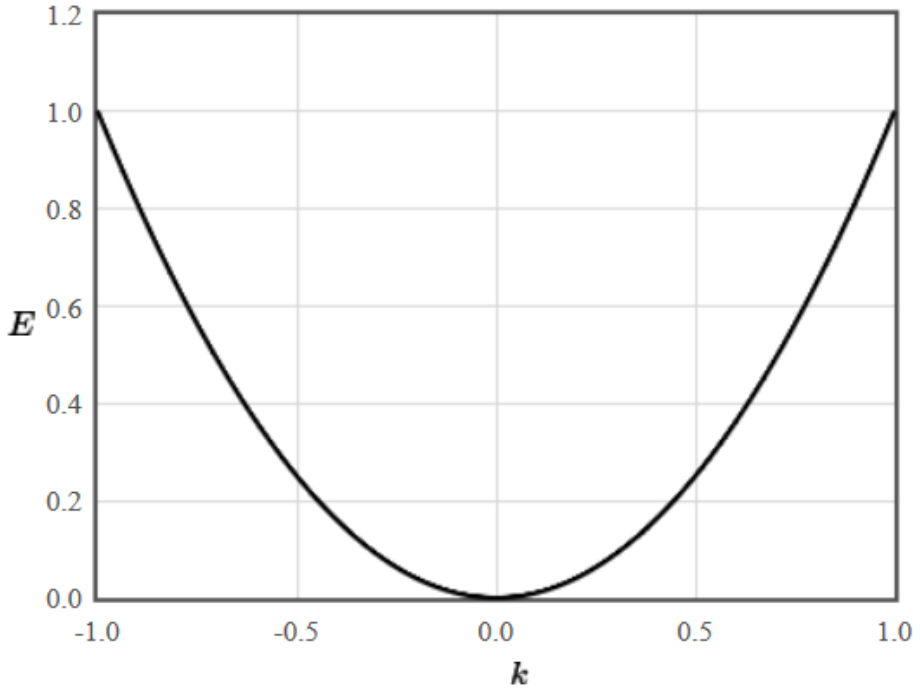
analog to the Planck curve for electrons in 1-d

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}

Empty lattice approximation

Free electrons cannot absorb photons

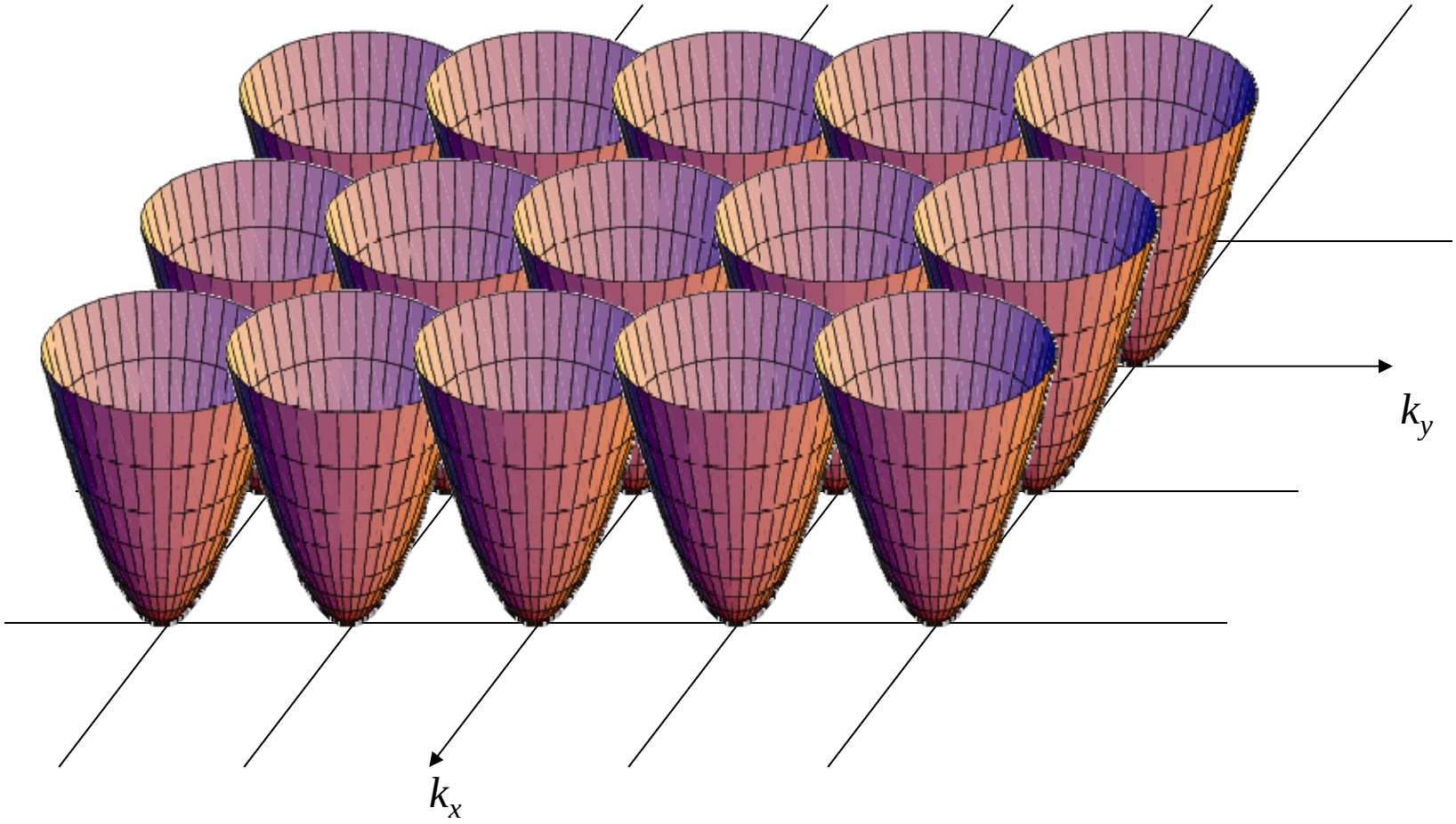


$$\hbar\vec{k}_f = \hbar\vec{k}_i + \hbar\vec{G}$$

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

Laue condition

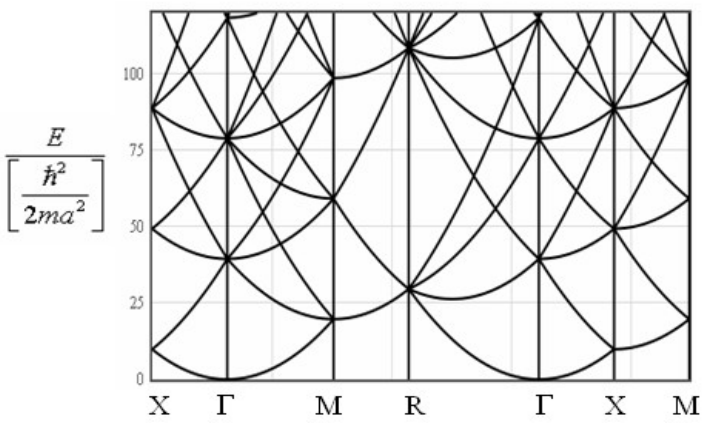
Empty lattice approximation



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

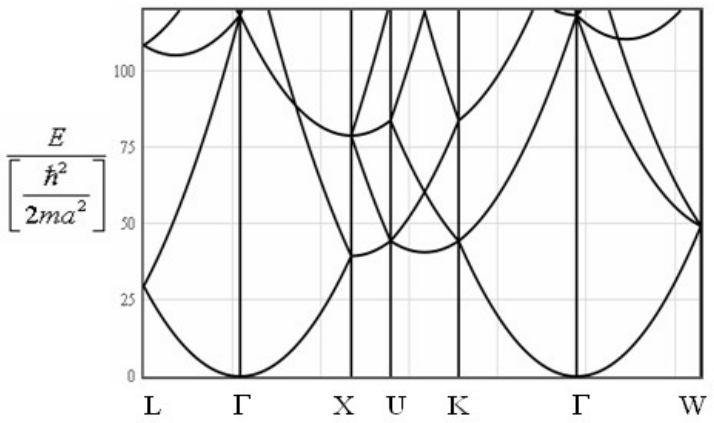
Empty lattice approximation

Simple cubic



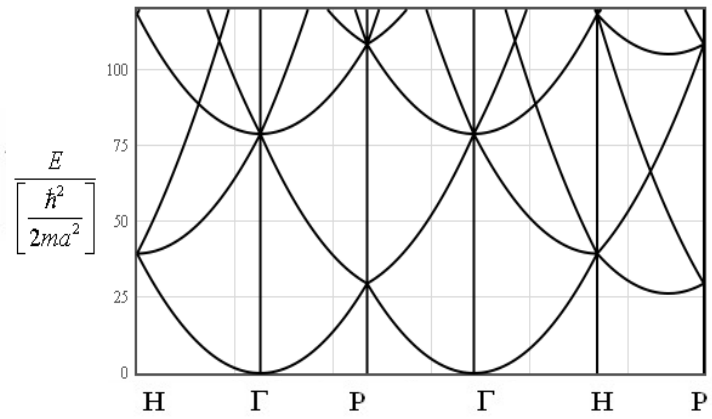
Choose a different order for the symmetry points

Face centered cubic

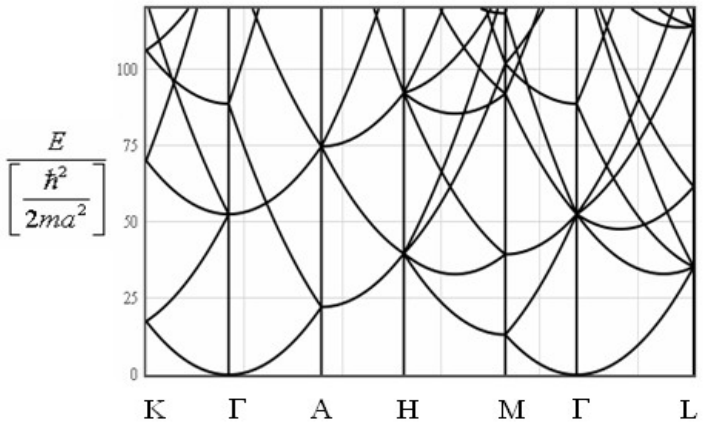


Choose a different order for the symmetry points

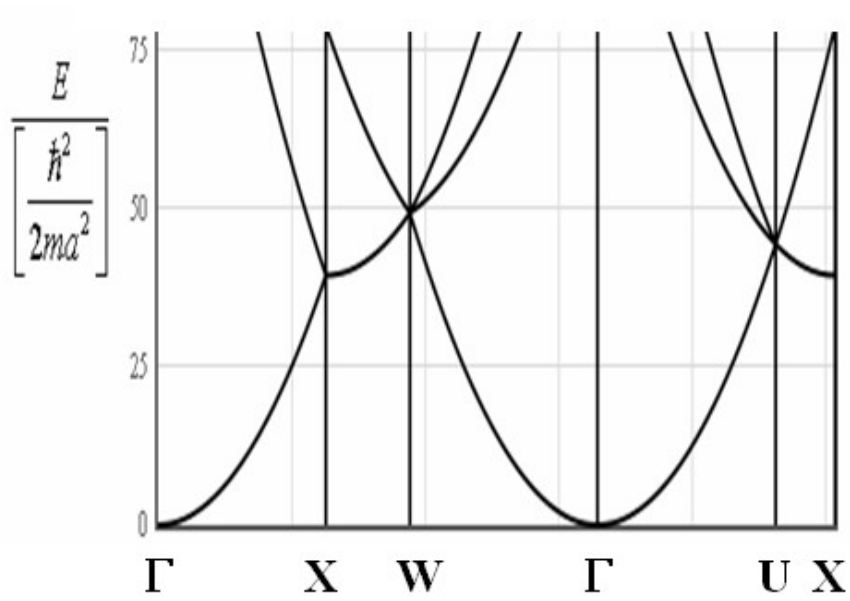
Body centered cubic

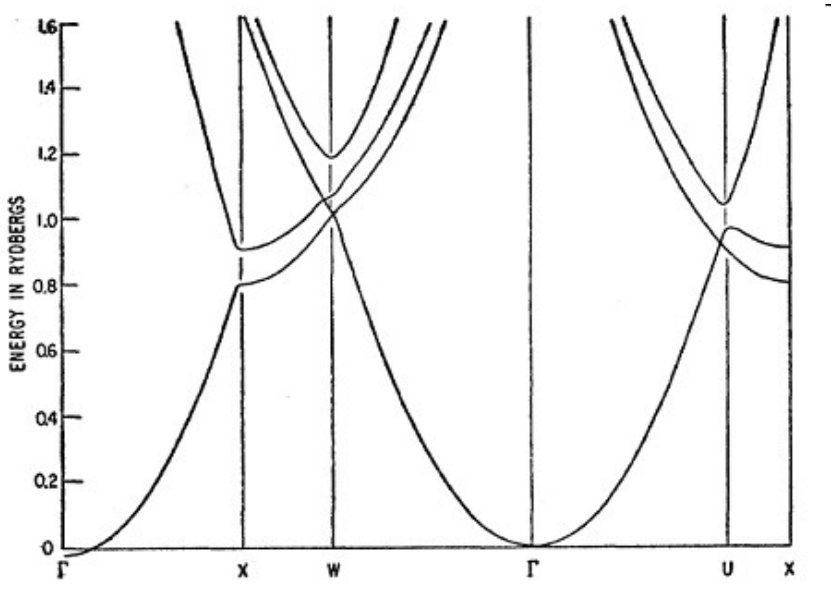


Hexagonal



Empty lattice approximation



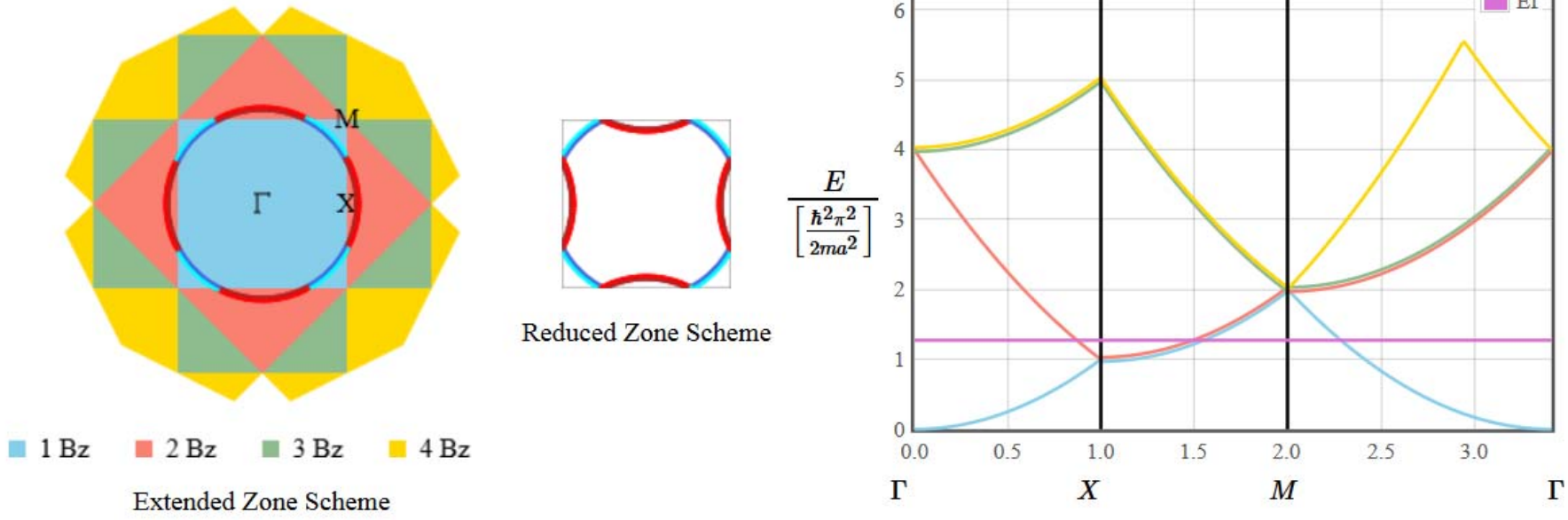


W. Harrison, Phys. Rev. 118 p. 1182 (1960)

aluminum

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