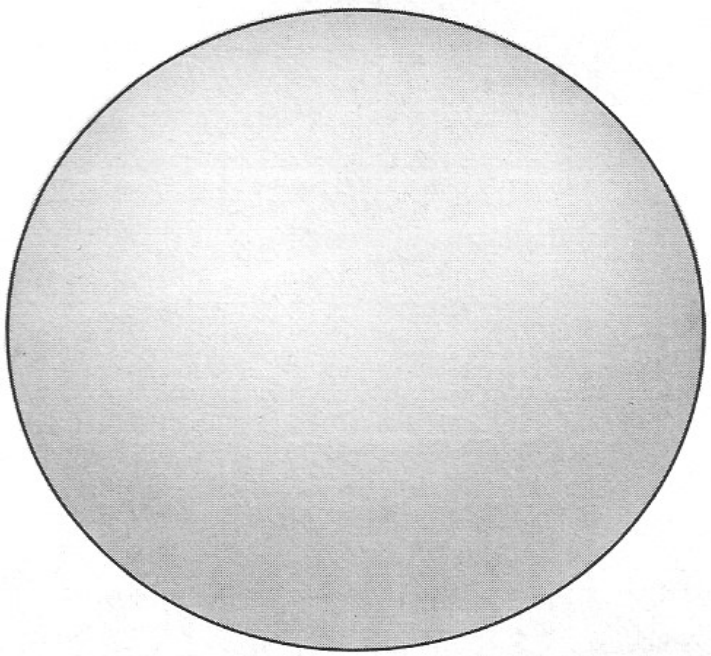
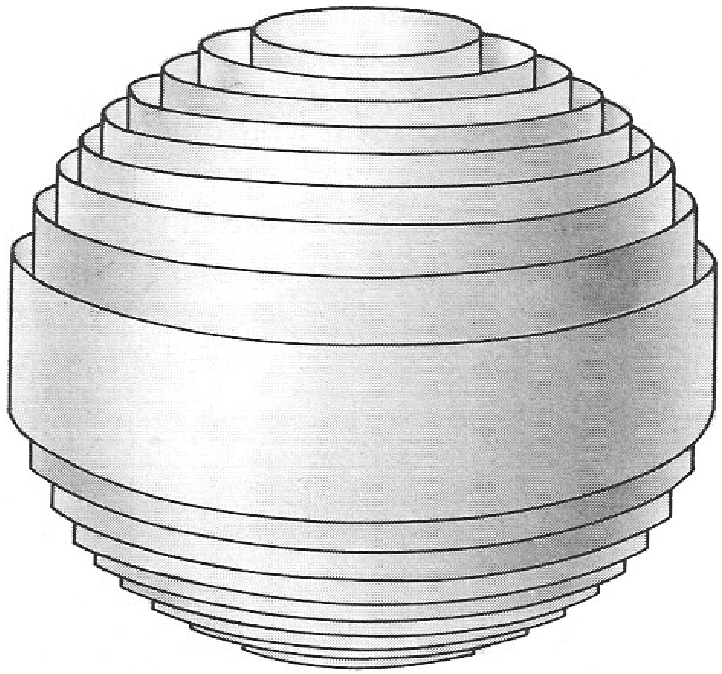
Fermi sphere in a magnetic field



$B = 0$

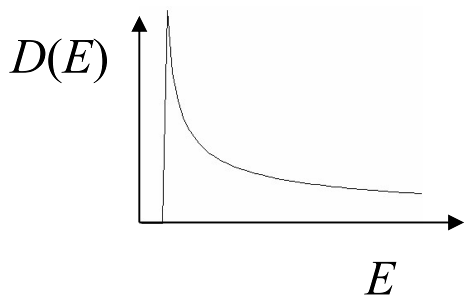


$B \neq 0$

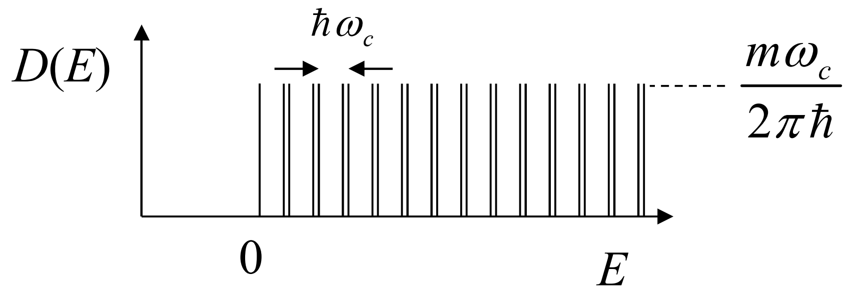
Landau cylinders

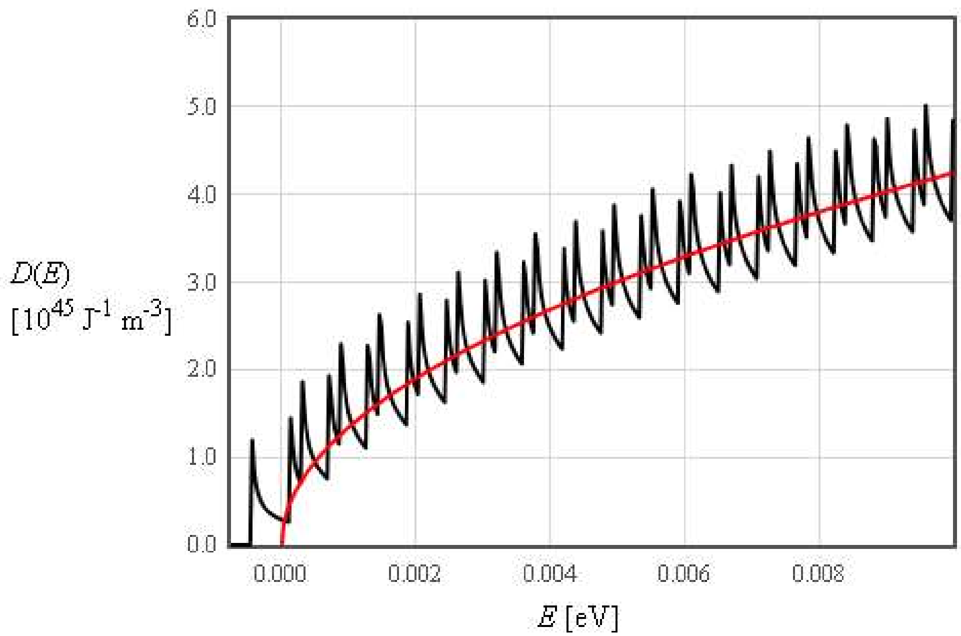
Density of states 3d

convolution of



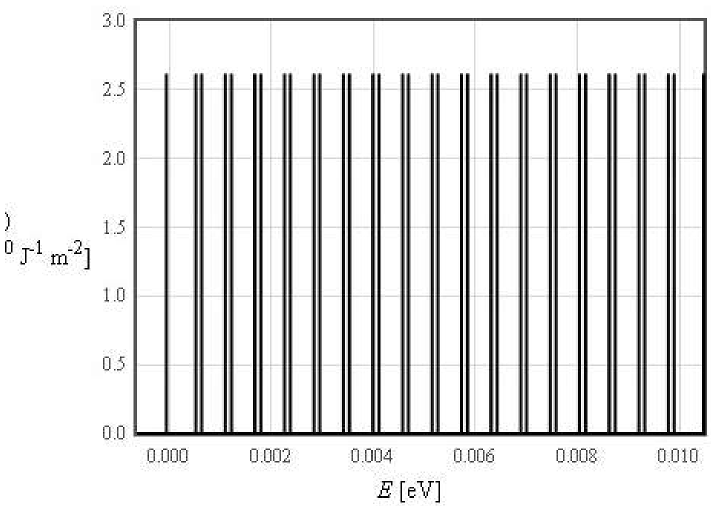
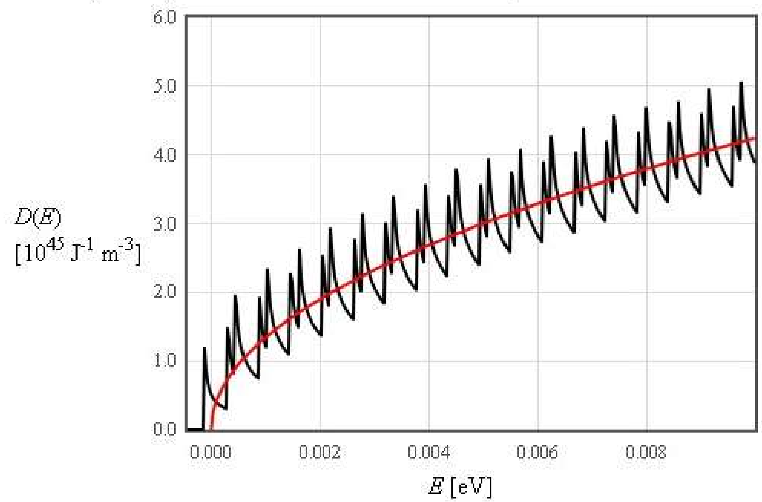
and





$$D(E) = \frac{(2m)^{3/2}\,\omega_c}{8\pi^2\hbar^2}\left(\sum_{v=0}^{\infty}\frac{H\left(E-\hbar\omega_c\left(v+\frac{1}{2}-g/4\right)\right)}{\sqrt{E-\hbar\omega_c\left(v+\frac{1}{2}-g/4\right)}}+\frac{H\left(E-\hbar\omega_c\left(v+\frac{1}{2}+g/4\right)\right)}{\sqrt{E-\hbar\omega_c\left(v+\frac{1}{2}+g/4\right)}}\right) \quad \mathrm{J^{-1}m^{-3}}$$

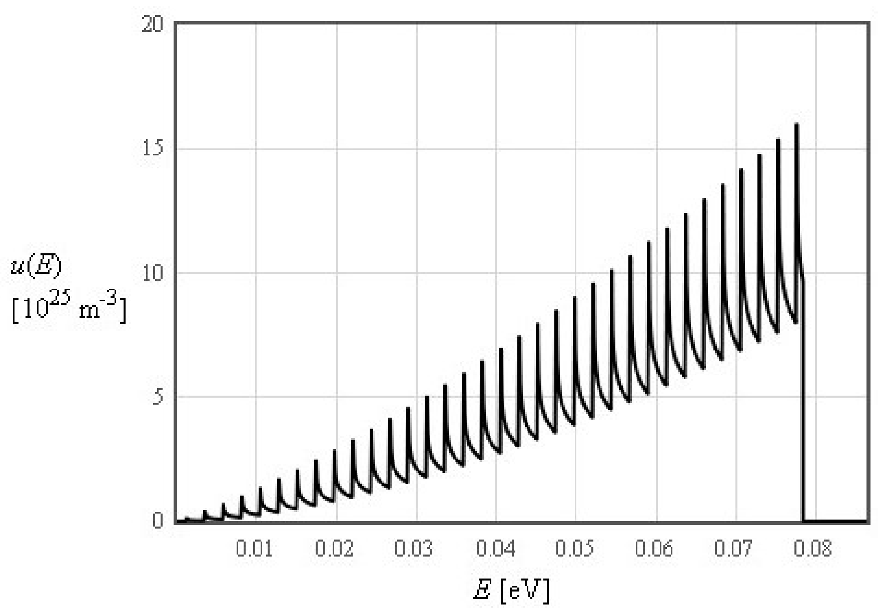
quation for free electrons a magnetic field in 2 and 3 dimensions.

2-D Schrödinger equation	3-D Schrödinger equation
$i\hbar\frac{d\psi}{dt}=\frac{1}{2m}\left(-i\hbar\nabla-\lvert e\rvert\vec{A}\right)^2\psi$	$i\hbar\frac{d\psi}{dt}=\frac{1}{2m}\left(-i\hbar\nabla-\lvert e\rvert\vec{A}\right)^2\psi$
$\psi=g_v(x)\exp\left(ik_y y\right)$ $g_v(x)$ is a harmonic oscillator wavefunction	$\psi=g_v(x)\exp\left(ik_y y\right)\exp\left(ik_z z\right)$ $g_v(x)$ is a harmonic oscillator wavefunction
$E=\hbar\omega_c\left(v+\frac{1}{2}\right)$ J $v=0,1,2,\cdots$ $\quad\omega_c=\frac{\lvert eB_z\rvert}{m}$	$E=\frac{\hbar^2k_z^2}{2m}+\hbar\omega_c\left(v+\frac{1}{2}\right)$ J $v=0,1,2,\cdots$ $\quad\omega_c=\frac{\lvert eB_z\rvert}{m}$
$\sum_{v=0}^{\infty}\delta\left(E-\hbar\omega_c\left(v+\frac{1}{2}\right)-\frac{g\mu_B}{2}B\right)+\delta\left(E-\hbar\omega_c\left(v+\frac{1}{2}\right)+\frac{g\mu_B}{2}B\right)$ $\mathrm{J^{-1}m^{-2}}$  Calculate DoS	$D(E)=\frac{(2m)^{3/2}\omega_c}{8\pi^2\hbar^2}\left(\sum_{v=0}^{\infty}\frac{H\left(E-\hbar\omega_c\left(v+\frac{1}{2}-g/4\right)\right)}{\sqrt{E-\hbar\omega_c\left(v+\frac{1}{2}-g/4\right)}}+\frac{H\left(E-\hbar\omega_c\left(v+\frac{1}{2}+g/4\right)\right)}{\sqrt{E-\hbar\omega_c\left(v+\frac{1}{2}+g/4\right)}}\right)$ $\mathrm{J^{-1}m^{-3}}$  Calculate DoS
$E_F=\hbar\omega\left(\mathrm{Int}\left(\frac{\pi\hbar n}{\ldots}\right)+\frac{1}{\ldots}\right)$	

Energy spectral density 3d

At $T = 0$

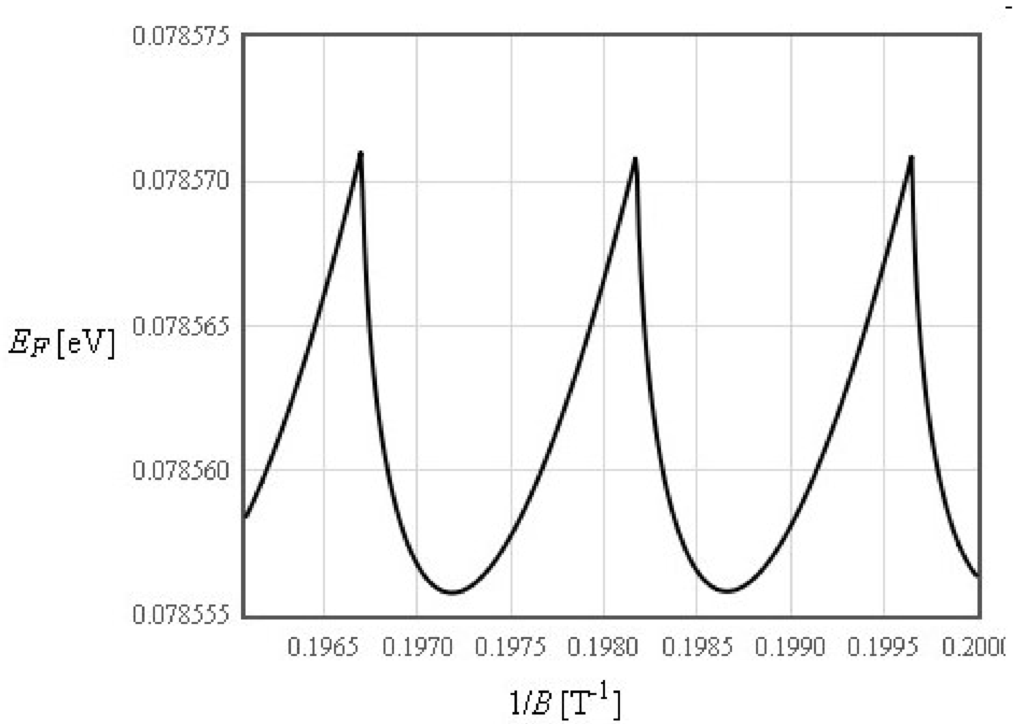
$$u(E) = ED(E)f(E)$$



$$u(T=0) = \int_{-\infty}^{E_F} ED(E)dE$$

Fermi energy 3d

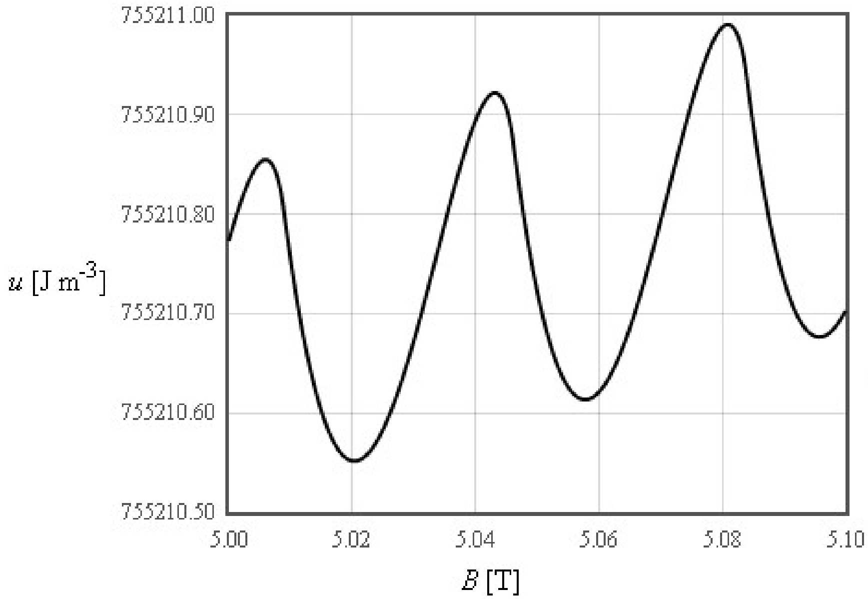
$$n = \int_{-\infty}^{E_F} D(E)dE$$



Periodic in 1/*B*

Internal energy 3d

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



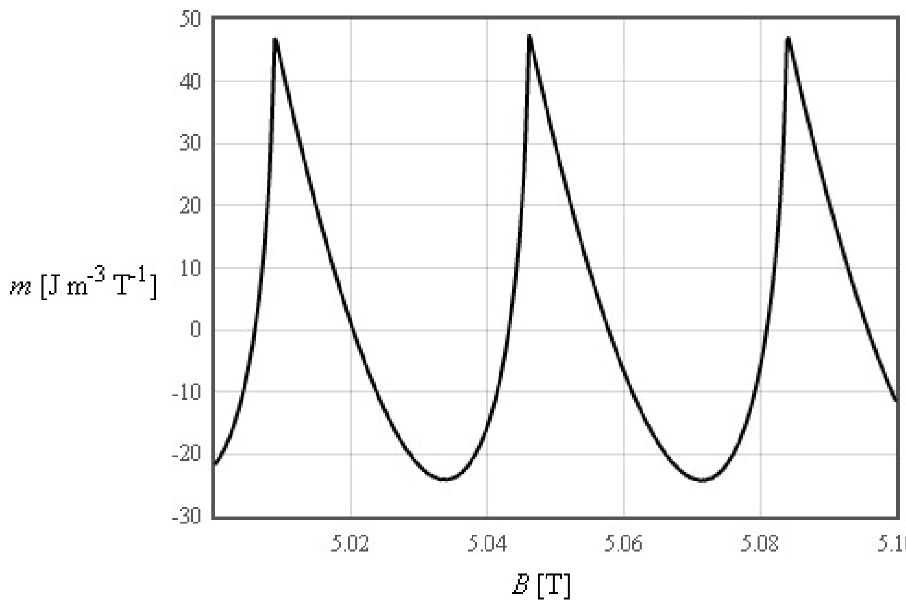
At $T = 0$

$$u = \frac{(2m)^{3/2}\omega_c}{4\pi^2\hbar^2} \sum_{\nu=0}^{\nu < \frac{E_F}{\hbar\omega_c} - \frac{1}{2}} \int_{\hbar\omega_c(\nu+\frac{1}{2})}^{E_F} \frac{E dE}{\sqrt{E - \hbar\omega_c(\nu + \frac{1}{2})}} \quad \text{J m}^{-3}$$

$$u = \frac{(2m)^{3/2}\omega_c}{6\pi^2\hbar^2} \sum_{\nu=0}^{\nu < \frac{E_F}{\hbar\omega_c} - \frac{1}{2}} \left(2\hbar\omega_c(\nu + \tfrac{1}{2}) + E_F\right)\sqrt{E_F - \hbar\omega_c(\nu + \tfrac{1}{2})} \quad \text{J m}^{-3}$$

Magnetization 3d

$$m = -\frac{du}{dB}$$



Periodic in $1/B$

At finite temperatures this function would be smoother

de Haas - van Alphen oscillations

Practically all properties are periodic in 1/*B*

Internal energy

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

Specific heat

$$c_v = \left(\frac{\partial u}{\partial T}\right)_{V=const}$$

Entropy

$$s = \int \frac{c_v}{T} dT$$

Helmholtz free energy

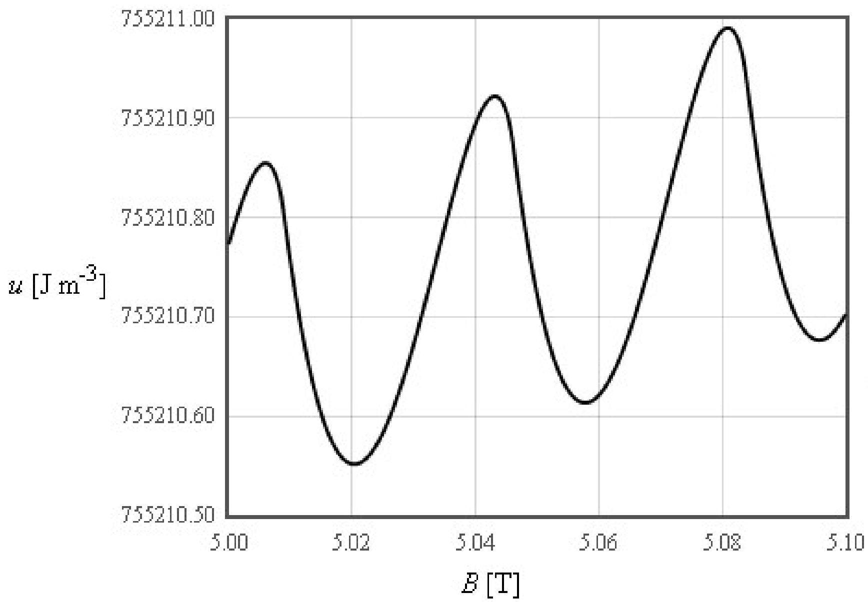
$$f = u - Ts$$

Pressure

$$P = -\left(\frac{\partial F}{\partial V}\right)_{T=const}$$

Bulk modulus

$$B = -V \frac{\partial P}{\partial V}$$

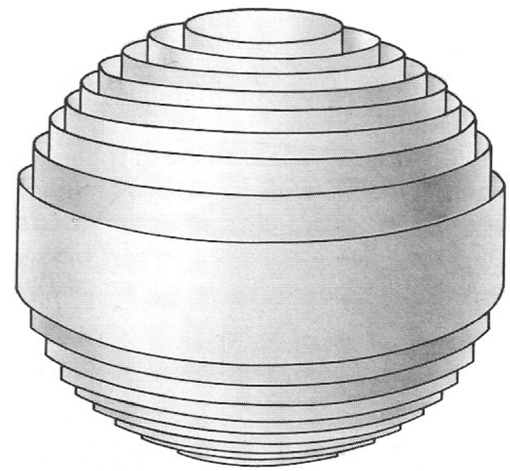


Magnetization

$$M = -\frac{dU}{dH}$$

Fermi sphere in a magnetic field

Cross sectional area $S = \pi k_F^2$



$$\hbar \omega_c \left(v + \tfrac{1}{2} \right) = \frac{\hbar^2 k_F^2}{2m}$$

$$\hbar \frac{eB_v}{m} \left(v + \tfrac{1}{2} \right) = \frac{\hbar^2 k_F^2}{2m}$$

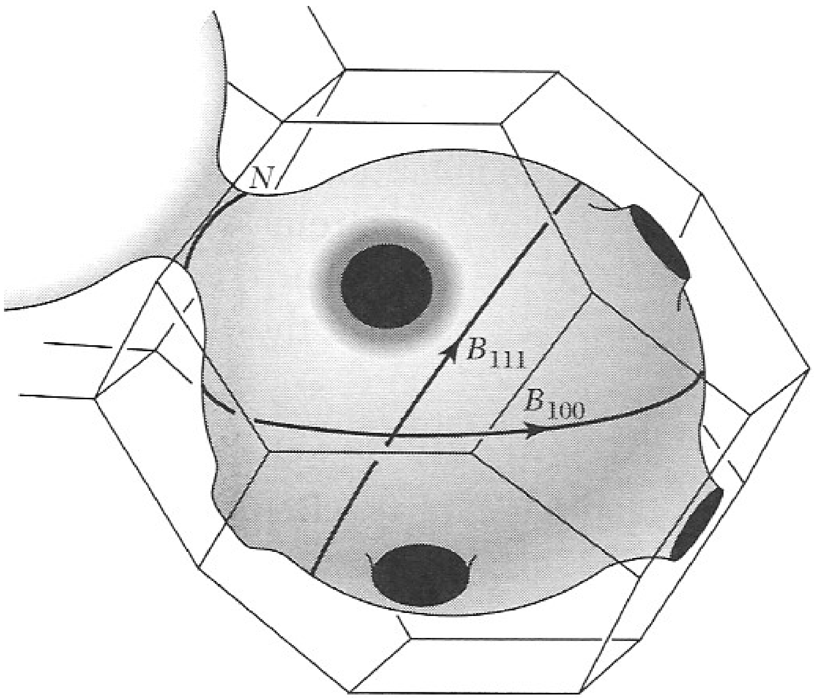
$$\frac{2\pi e}{\hbar} \left(v + 1 + \tfrac{1}{2} \right) = \frac{S}{B_{v+1}} \qquad \frac{2\pi e}{\hbar} \left(v + \tfrac{1}{2} \right) = \frac{S}{B_v}$$

Subtract right from left

$$S \left(\frac{1}{B_{v+1}} - \frac{1}{B_v} \right) = \frac{2\pi e}{\hbar}$$

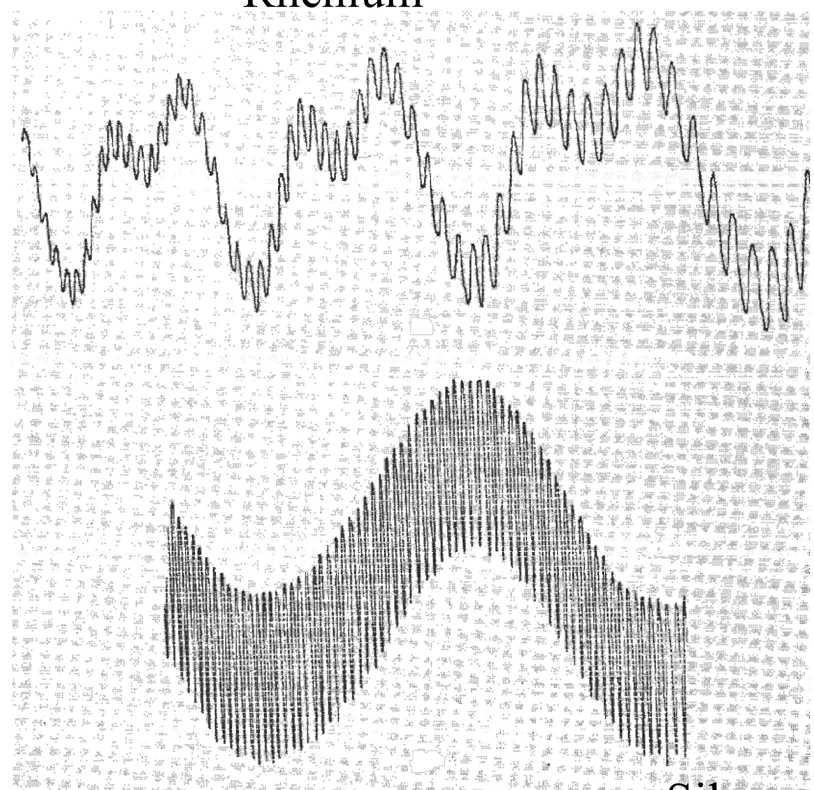
From the periodic of the oscillations, you can determine the cross sectional area *S*.

Experimental determination of the Fermi surface



Kittel

Rhenium

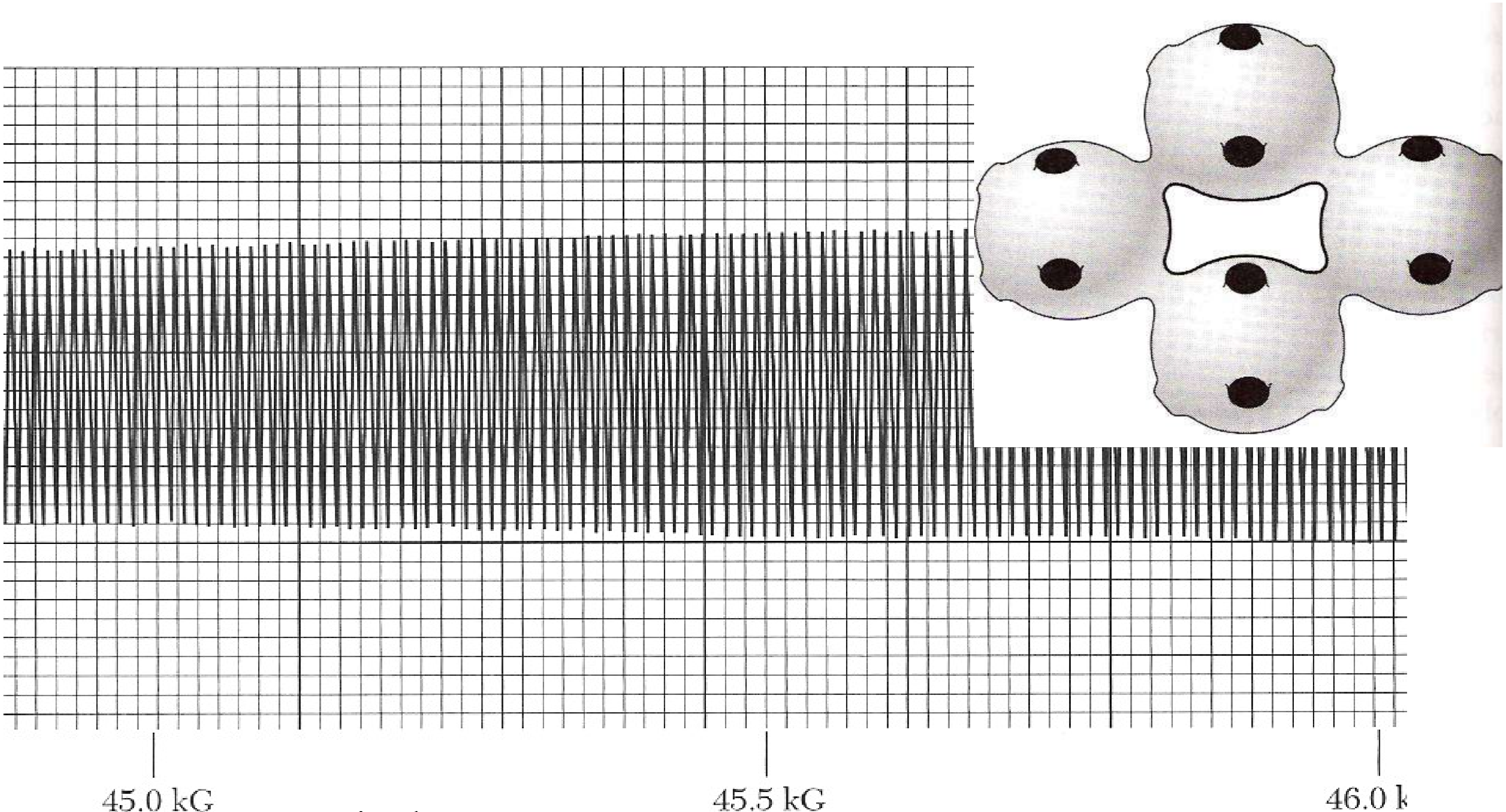


Silver

de Haas - van Alphen

De Haas - van Alphen effect

The magnetic moment of gold oscillates periodically with $1/B$



Kittel

Classical linear response theory

Fourier transforms
Impulse response functions (Green's functions)
Generalized susceptibility
Causality
Kramers-Kronig relations
Fluctuation - dissipation theorem
Dielectric function
Optical properties of solids

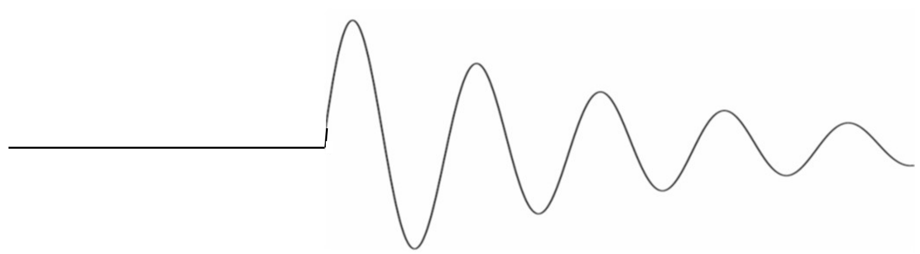
Impulse response function (Green's functions)

A Green's function is the solution to a linear differential equation for a δ-function driving force

For instance,
$$m\frac{d^2 g}{dt^2} + b\frac{dg}{dt} + kg = \delta(t)$$

has the solution

$$g(t) = \frac{1}{m}\exp\left(\frac{-bt}{2m}\right)\sin\left(\frac{\sqrt{4mk - b^2}}{2m}t\right) \qquad t > 0$$



Green's functions

A driving force *f* can be thought of a being built up of many delta functions after each other.

$$f(t) = \int \delta\left(t - t'\right) f\left(t'\right) dt'$$

By superposition, the response to this driving function is superposition,

$$u(t) = \int g(t - t') f(t') dt'$$

For instance, $$m\frac{d^2u}{dt^2} + b\frac{du}{dt} + ku = f(t)$$

has the solution

$$u(t) = \int_{-\infty}^{\infty} \frac{1}{m} \exp\left(\frac{-b\left(t - t'\right)}{2m}\right) \sin\left(\frac{\sqrt{4mk - b^2}}{2m}\left(t - t'\right)\right) f(t') dt'$$

Green's function converts a differential equation into an integral equation

Generalized susceptibility

A driving function *f* causes a response *u*

If the driving force is sinusoidal,

$$f(t) = F_0 e^{i\omega t}$$

The response will also be sinusoidal.

$$u(t) = \int g(t-t') f(t') dt' = \int g(t-t') F_0 e^{i\omega t'} dt'$$

The generalized susceptibility at frequency ω is

$$\chi(\omega) = \frac{u}{f} = \frac{\int g(t-t') e^{i\omega t'} dt'}{e^{i\omega t}}$$

Generalized susceptibility

$$\chi(\omega) = \frac{u}{f} = \frac{\int g(t-t')e^{i\omega t'}dt'}{e^{i\omega t}}$$

Since the integral is over t', the factor with t can be put in the integral.

$$\chi(\omega) = \int g(t-t')e^{-i\omega(t-t')}dt'$$

Change variables to $\tau = t - t'$

$$\chi(\omega) = \int g(\tau)e^{-i\omega\tau}d\tau$$

The susceptibility is the Fourier transform (notation [1,-1]) of the Green's function.

$$g(t) = \frac{1}{2\pi}\int \chi(\omega)e^{i\omega t}d\omega$$

Fourier Transforms

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

↑

The Fourier transform of $f(r)$.

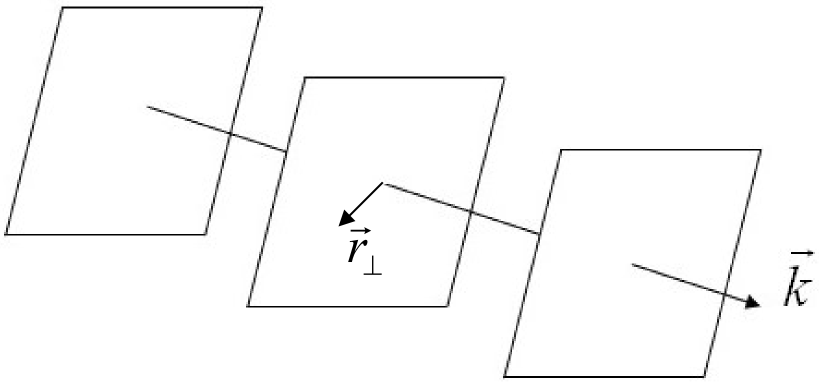
All information about $f(r)$ is contained in its Fourier transform.
All information about $F(k)$ is contained in $f(r)$.

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

d is the number of dimensions

Fourier Transforms: plane waves

Plane waves have the form: $\exp\left(i\vec{k}\cdot\vec{r}\right)=\cos\left(\vec{k}\cdot\vec{r}\right)+i\sin\left(\vec{k}\cdot\vec{r}\right)$



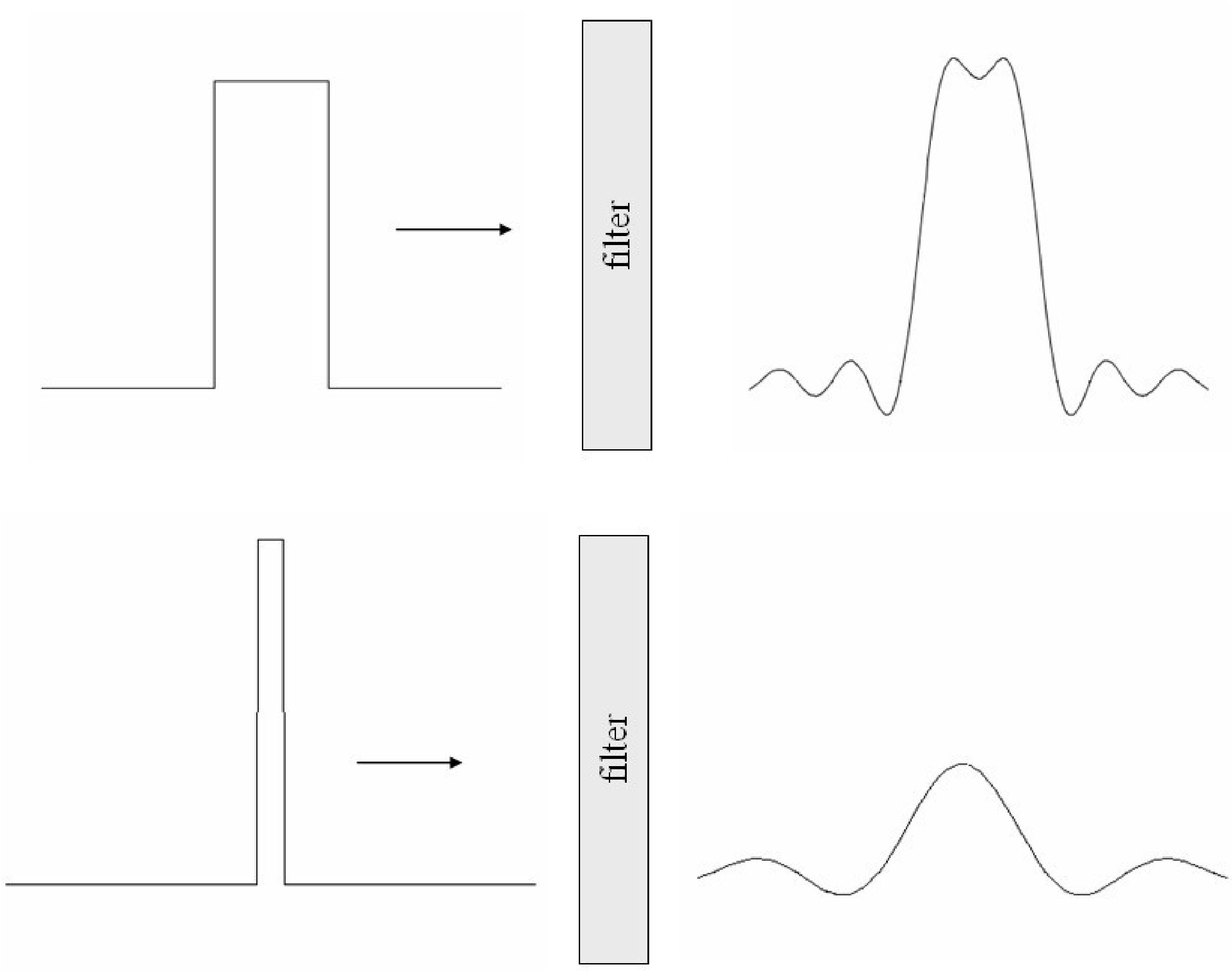
$$\exp\left(i\vec{k}\cdot\left(\vec{r}+\vec{r}_{\perp}\right)\right)=\exp\left(i\vec{k}\cdot\vec{r}\right)$$

Often convenient to work with functions expressed in terms of plane waves

$$f\left(\vec{r}\right)=\sum_{\vec{G}}F_{\vec{G}}\exp\left(i\vec{G}\cdot\vec{r}\right)$$ Periodic functions

$$f\left(\vec{r}\right)=\int F(\vec{k})\exp\left(i\vec{k}\cdot\vec{r}\right)d\vec{k}$$ Any functions

Fourier Transforms



Notation

[a,b]

$$F_{[a,b]}(\vec{k}) = \sqrt{\frac{|b|^d}{(2\pi)^{d(1-a)}}} \int f(\vec{r}) \exp\left(ib\vec{k}\cdot\vec{r}\right) d\vec{r}$$

$$f(\vec{r}) = \sqrt{\frac{|b|^d}{(2\pi)^{d(1+a)}}} \int F_{[a,b]}(\vec{k}) \exp\left(-ib\vec{k}\cdot\vec{r}\right) d\vec{k}$$

MathWorld

Notation

[-1,-1]

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

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

[1,-1]

$$F(\vec{k}) = \int f(\vec{r}) \exp\left(-i\vec{k} \cdot \vec{r}\right) d\vec{r}$$

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

Matlab

[0,-1]

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

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

Evertz, Mathematica uses [0,1]

[0,-2π]

$$F(\vec{q}) = \int f(\vec{r}) \exp\left(-i2\pi\vec{q} \cdot \vec{r}\right) d\vec{r}$$

$$f(\vec{r}) = \int F(\vec{q}) \exp\left(i2\pi\vec{q} \cdot \vec{r}\right) d\vec{q}$$

$$\lambda = \frac{1}{|\vec{q}|}$$

Engineering literature