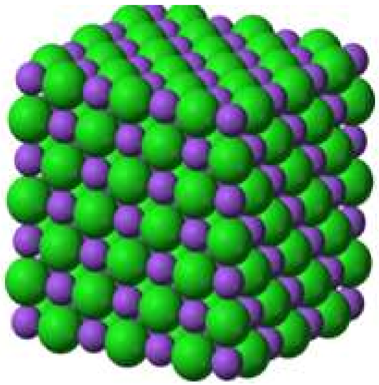
NaCl



2 atoms/unit cell

6 equations

3 acoustic and
3 optical branches

x - Richtung:

$$M_1 \frac{d^2 u^x_{nml}}{dt^2} = C\left(-2u^x_{nml} + v^x_{(n-1)m(l-1)} + v^x_{n(m-1)l}\right)$$

$$M_2 \frac{d^2 v^x_{nml}}{dt^2} = C\left(-2v^x_{nml} + u^x_{(n+1)m(l+1)} + u^x_{n(m+1)l}\right)$$

y - Richtung:

$$M_1 \frac{d^2 u^y_{nml}}{dt^2} = C\left(-2u^y_{nml} + v^y_{(n-1)(m-1)l} + v^y_{nm(l-1)}\right)$$

$$M_2 \frac{d^2 v^y_{nml}}{dt^2} = C\left(-2v^y_{nml} + u^y_{(n+1)(m+1)l} + u^y_{nm(l+1)}\right)$$

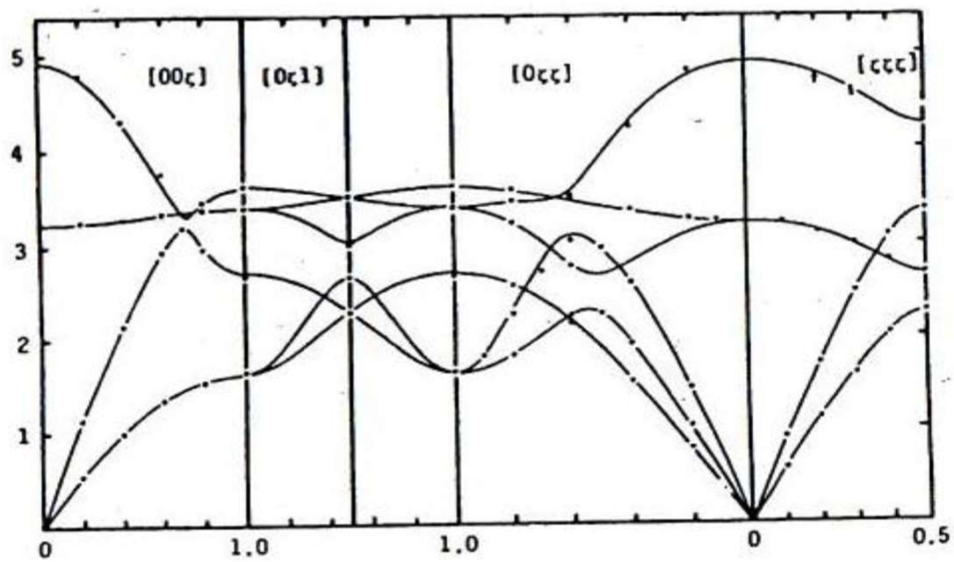
z - Richtung:

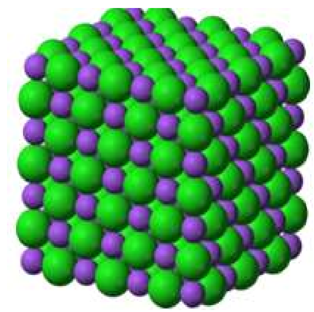
$$M_1 \frac{d^2 u^z_{nml}}{dt^2} = C\left(-2u^z_{nml} + v^z_{n(m-1)(l-1)} + v^z_{(n-1)ml}\right)$$

$$M_2 \frac{d^2 v^z_{nml}}{dt^2} = C\left(-2v^z_{nml} + u^z_{n(m+1)(l+1)} + u^z_{(n+1)ml}\right)$$

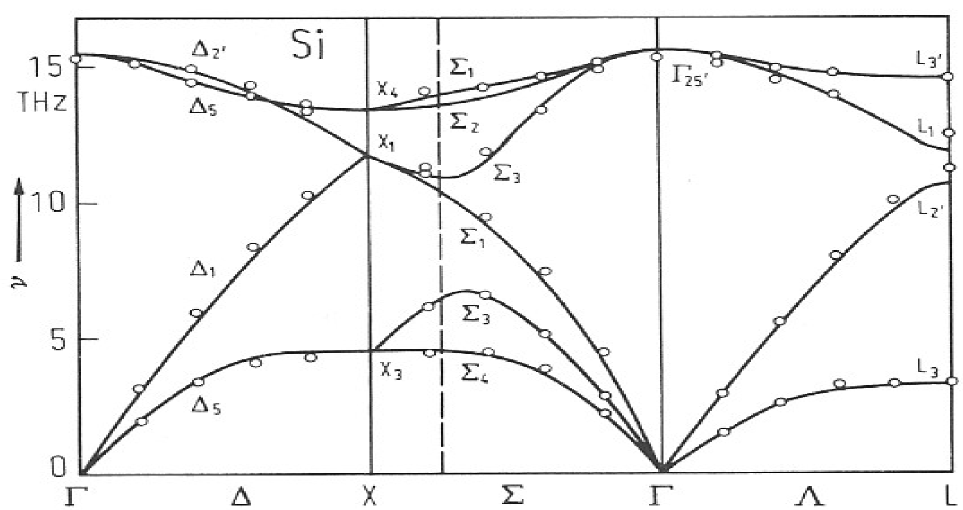
$$u^x_{nml} = u^x_{\vec{k}} \exp\left(i\left(\vec{k}\cdot\vec{a}_1 + \vec{k}\cdot\vec{a}_2 + \vec{k}\cdot\vec{a}_3 - \omega t\right)\right) \qquad v^x_{nml} = v^x_{\vec{k}} \exp\left(i\left(\vec{k}\cdot\vec{a}_1 + \vec{k}\cdot\vec{a}_2 + \vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

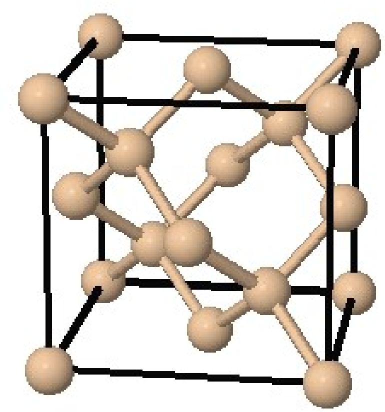
Two atoms per primitive unit cell





NaCl



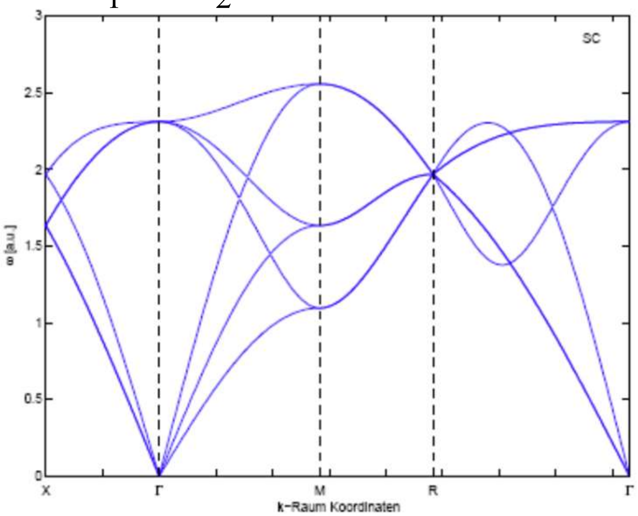


Si

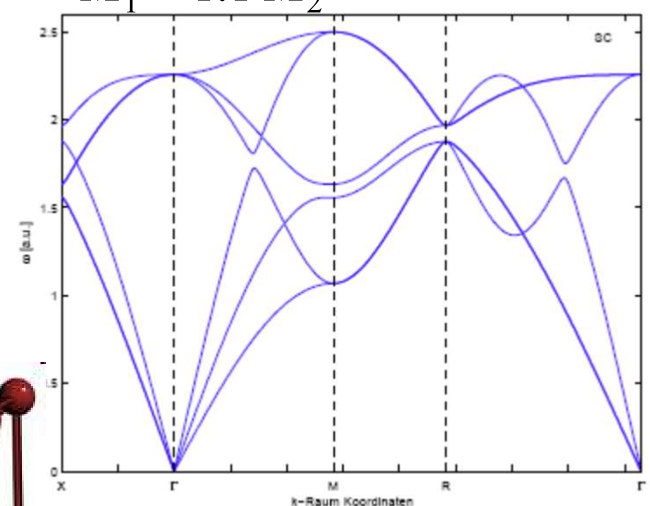
CsCl

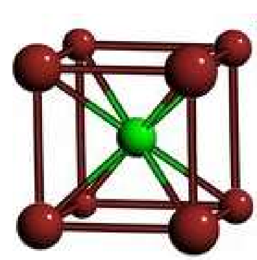
Hannes Brandner

$M_1 = M_2$

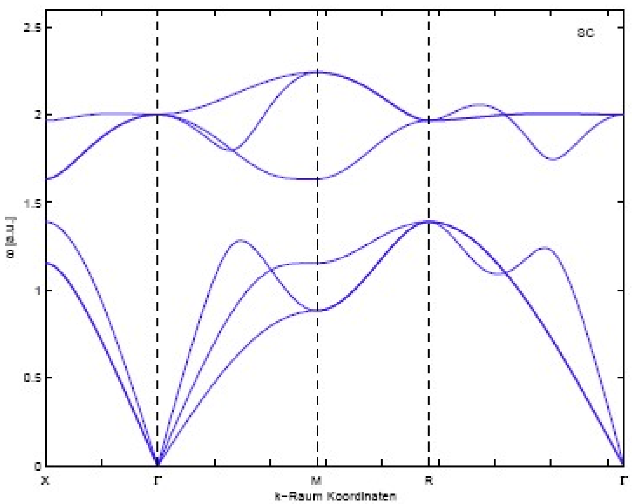


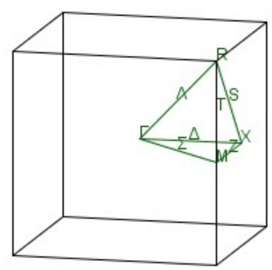
$M_1 = 1.1\ M_2$



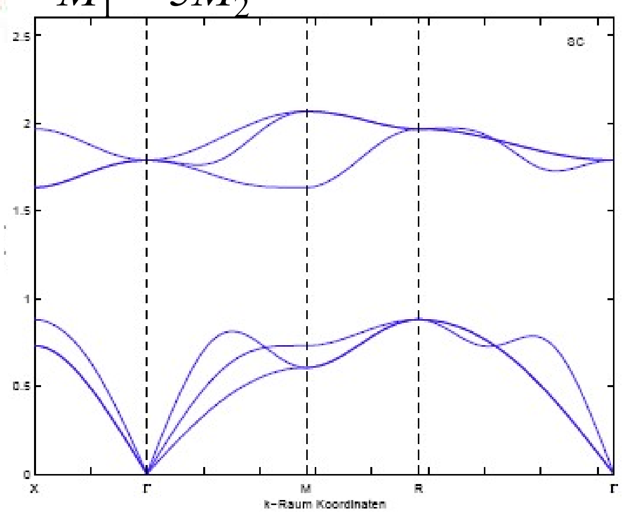


$M_1 = 2M_2$



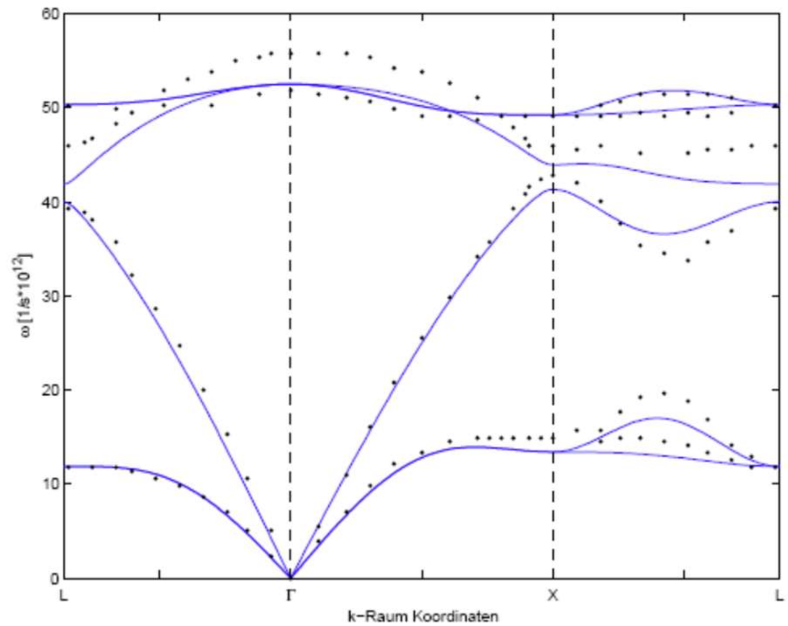


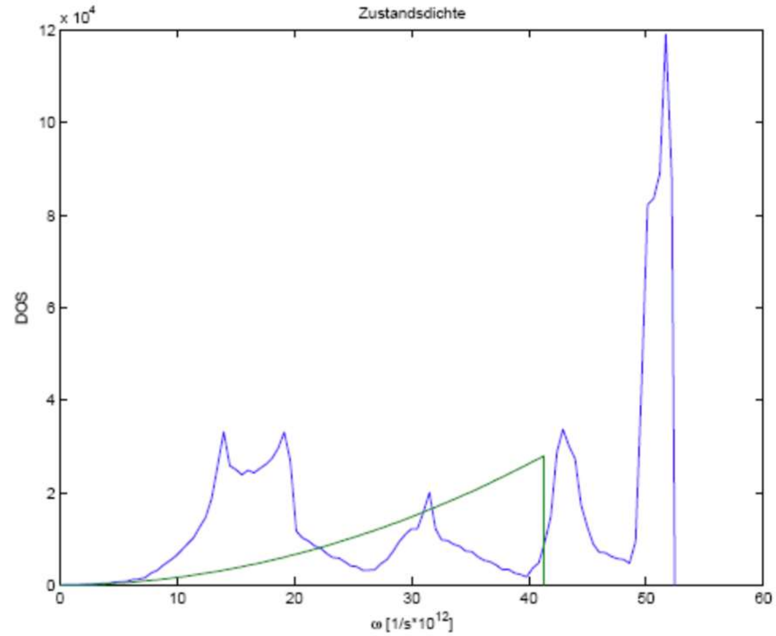
$M_1 = 5M_2$

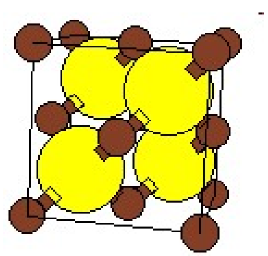


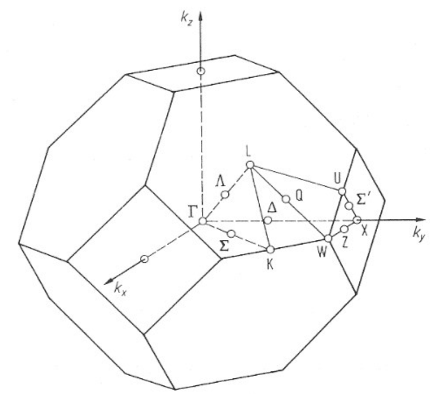
GaAs

Hannes Brandner









Phonon quasiparticle lifetime

Phonons are the eigenstates of the linearized equations, not the full equations.

Phonons have a finite lifetime that can be calculated by Fermi's golden rule.

$$\Gamma_{i \to f} = \frac{2\pi}{\hbar} \left| \langle f | H_{ph-ph} | i \rangle \right|^2 \delta\left(E_f - E_i\right)$$

Occupation is determined by a master equation (not the Bose-Einstein function).

$$\begin{bmatrix} \frac{dP_0}{dt} \\ \frac{dP_1}{dt} \\ \vdots \\ \frac{dP_N}{dt} \end{bmatrix} = \begin{bmatrix} -\sum\limits_{i \neq 0} \Gamma_{0 \to i} & \Gamma_{1 \to 0} & \cdots & \Gamma_{N \to 0} \\ \Gamma_{0 \to 1} & -\sum\limits_{i \neq 1} \Gamma_{1 \to i} & \cdots & \Gamma_{N \to 1} \\ \vdots & \vdots & \ddots & \vdots \\ \Gamma_{0 \to N} & \Gamma_{1 \to N} & \cdots & -\sum\limits_{i \neq N} \Gamma_{N \to i} \end{bmatrix} \begin{bmatrix} P_0 \\ P_1 \\ \vdots \\ P_N \end{bmatrix}$$

Acoustic attenuation

The amplitude of a monocromatic sound wave decreases as the wave propagates through the crystal as the phonon quasiparticles decay into phonons with other frequencies and directions.

Magnetism

Diamagnetism:
A dissipationless current is induced by a magnetic field that opposes the applied field.

Paramagnetism:
An applied field aligns the magnetic moments in the material making the field in the material larger than the applied field.

$$\vec{M} = \chi \vec{H}$$

Diamagnetic susceptibility	
Copper	-9.8×10^{-6}
Diamond	-2.2×10^{-5}
Gold	-3.6×10^{-5}
Lead	-1.7×10^{-5}
Nitrogen	-5.0×10^{-9}
Silicon	-4.2×10^{-6}
water	-9.0×10^{-6}
bismuth	-1.6×10^{-4}

Paramagnetic susceptibility	
Aluminum	2.3×10^{-5}
Calcium	1.9×10^{-5}
Magnesium	1.2×10^{-5}
Oxygen	2.1×10^{-6}
Platinum	2.9×10^{-4}
Tungsten	6.8×10^{-5}

Magnetism

magnetic intensity

$$\vec{B} = \mu_0 \left(\vec{H} + \vec{M} \right)$$

magnetic induction field

$$\vec{M} = \chi \vec{H}$$

magnetization

χ is the magnetic susceptibility

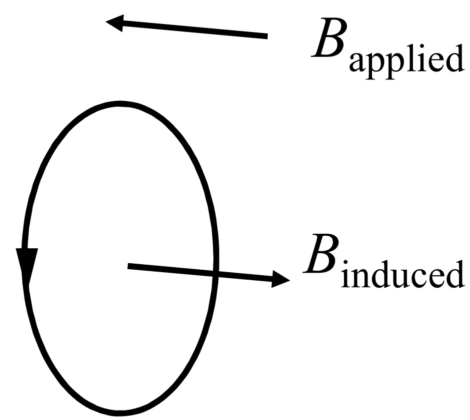
$\chi < 0$ diamagnetic

$\chi > 0$ paramagnetic

χ is typically small (10^{-5}) so $B \approx \mu_0 H$

Diamagnetism

A free electron in a magnetic field will travel in a circle



The magnetic created by the current loop is opposite the applied field.

Diamagnetism

Dissipationless currents are induced in a diamagnet that generate a field that opposes an applied magnetic field.

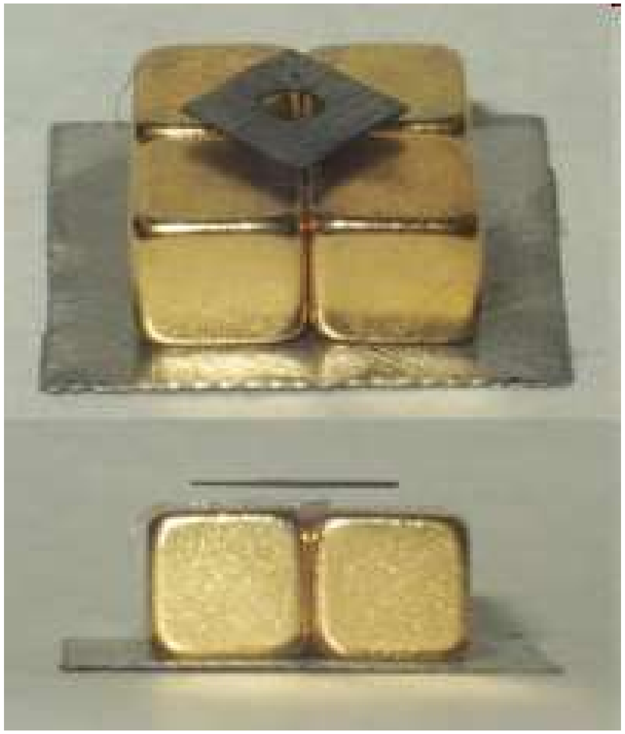
Current flow without dissipation is a quantum effect. There are no lower lying states to scatter into. This creates a current that generates a field that opposes the applied field.

$\chi = -1$ superconductor (perfect diamagnet)

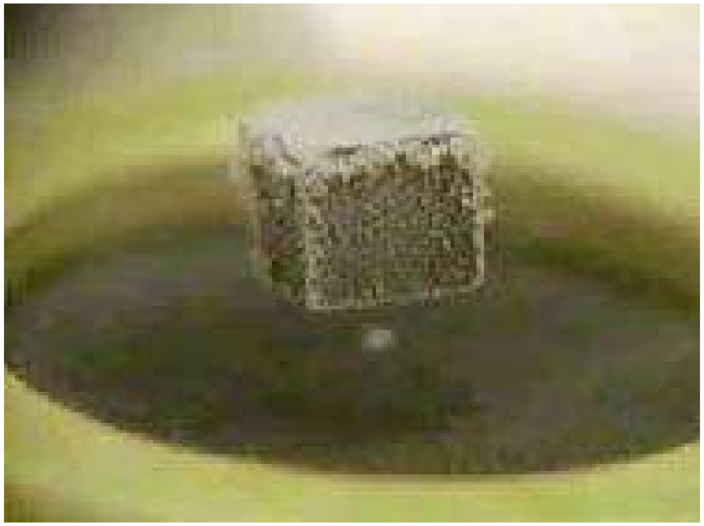
$\chi \sim -10^{-6}$ - 10^{-5} normal materials

Diamagnetism is always present but is often overshadowed by some other magnetic effect.

Levitating diamagnets



Levitating pyrolytic carbon



NOT: Lenz's law

$$V = -\frac{d\Phi}{dt}$$

Diamagnetism

A dissipationless current is induced by a magnetic field that opposes the applied field.

$$\vec{M} = \chi \vec{H}$$

Diamagnetic susceptibility	
Copper	-9.8×10^{-6}
Diamond	-2.2×10^{-5}
Gold	-3.6×10^{-5}
Lead	-1.7×10^{-5}
Nitrogen	-5.0×10^{-9}
Silicon	-4.2×10^{-6}
water	-9.0×10^{-6}
bismuth	-1.6×10^{-4}

Most stable molecules have a closed shell configuration and are diamagnetic.

Paramagnetism

Materials that have a magnetic moment are paramagnetic.

An applied field aligns the magnetic moments in the material making the field in the material larger than the applied field.

The internal field is zero at zero applied field (random magnetic moments).

$$\vec{M} = \chi \vec{H}$$

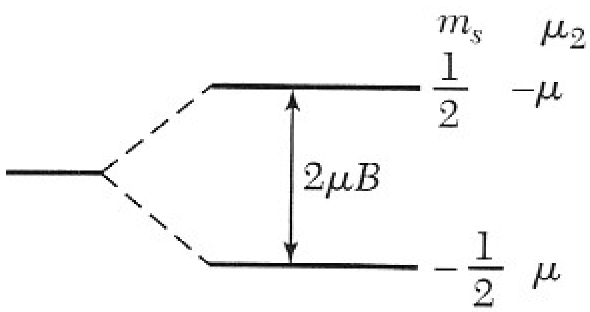
Paramagnetic susceptibility	
Aluminum	2.3×10^{-5}
Calcium	1.9×10^{-5}
Magnesium	1.2×10^{-5}
Oxygen	2.1×10^{-6}
Platinum	2.9×10^{-4}
Tungsten	6.8×10^{-5}

Boltzmann factors

To take the average value of quantity *A*

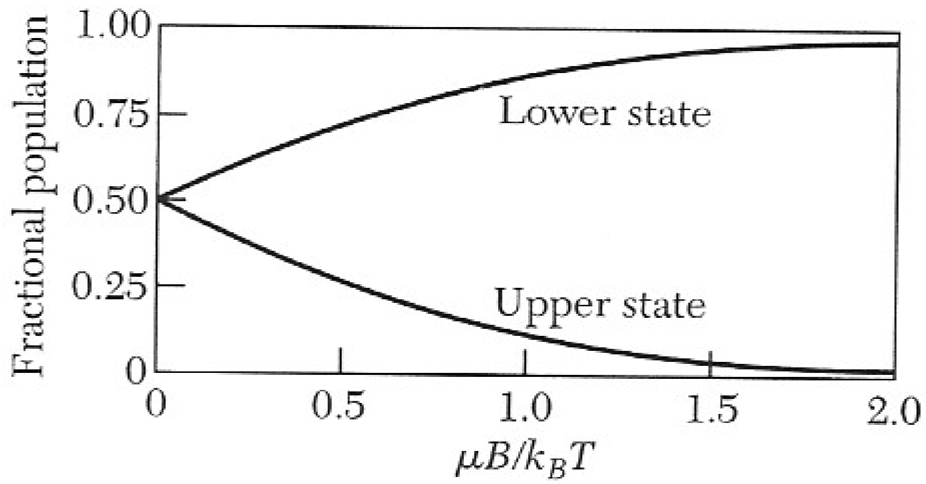
$$\langle A \rangle = \frac{\sum_i A_i e^{-E_i / k_B T}}{\sum_i e^{-E_i / k_B T}}$$

Spin populations



$$\frac{N_1}{N} = \frac{\exp(\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$

$$\frac{N_2}{N} = \frac{\exp(-\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$

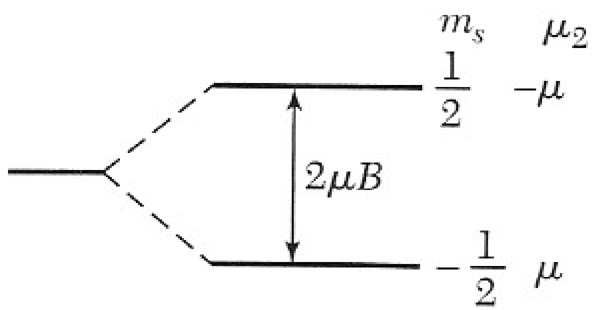


$$M = (N_1 - N_2)\mu$$

$$= N\mu \frac{\exp(\mu B / k_B T) - \exp(-\mu B / k_B T)}{\exp(\mu B / k_B T) + \exp(-\mu B / k_B T)}$$

$$= N\mu \tanh\left(\frac{\mu B}{k_B T}\right)$$

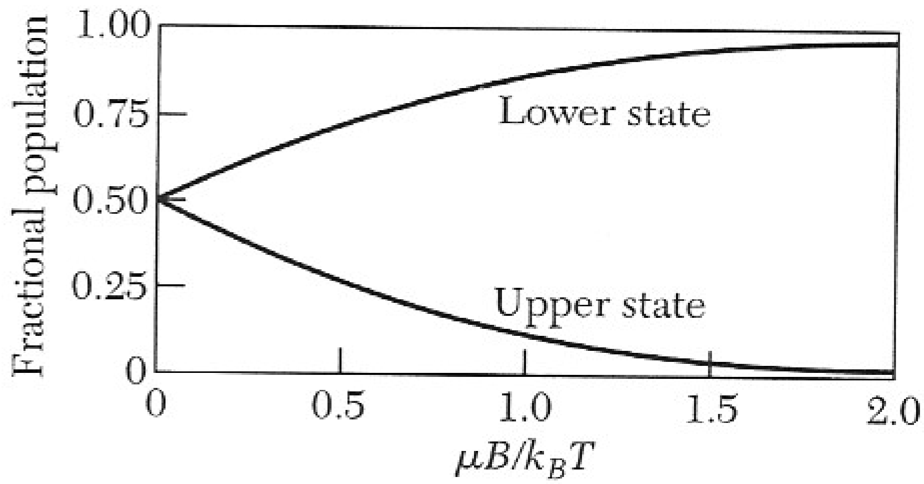
Paramagnetism, spin 1/2

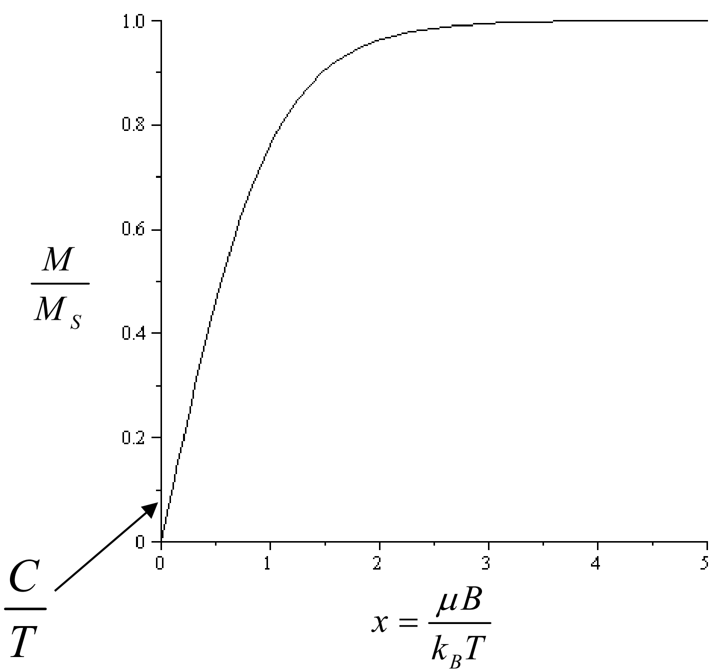


$$M = N\mu \tanh\left(\frac{\mu B}{k_B T}\right) \approx \frac{N\mu^2 B}{k_B T} = \frac{CB}{T}$$

for $\mu B << k_B T$

Curie law





$$\chi \approx \frac{C}{T}$$