Phonons and Magnons

Phonons

N_{atom} atoms in crystal

$3N_{atom}$ normal modes

p atoms in the basis

N_{atom}/p unit cells

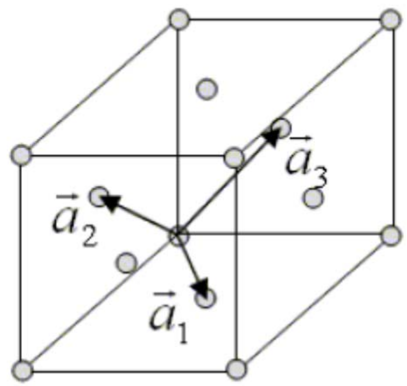
N_{atom}/p translational symmetries

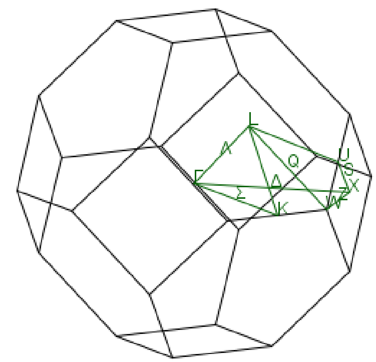
N_{atom}/p k-vectors

$3p$ modes for every k vector

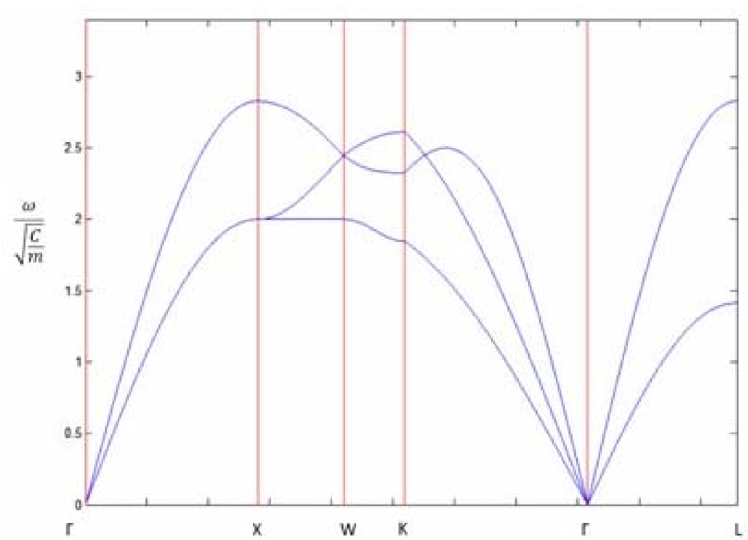
3 acoustic branches and $3p$-3 optical branches

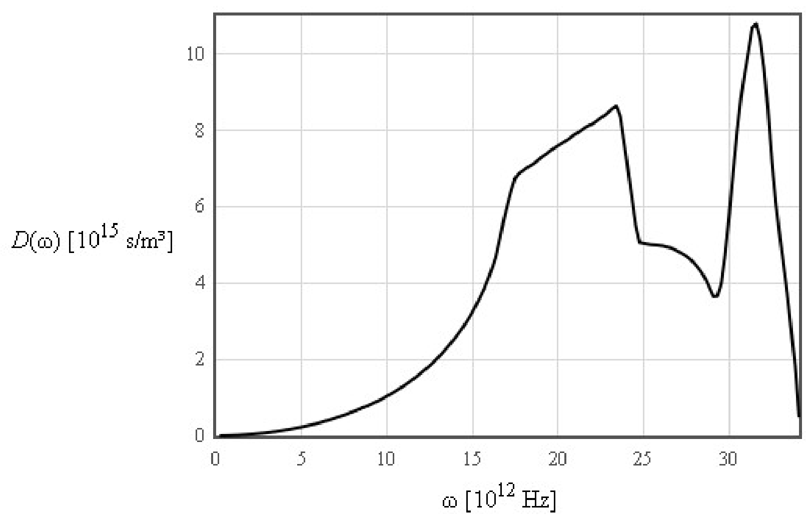
fcc phonons



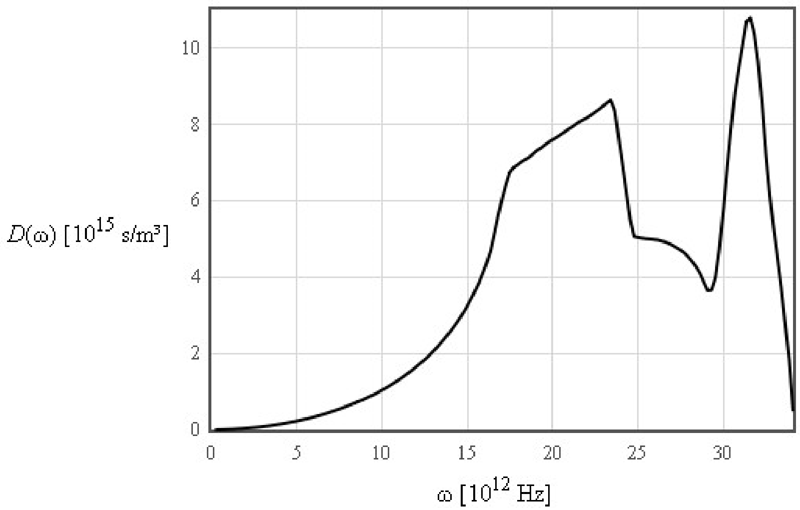


3*N* degrees of freedom

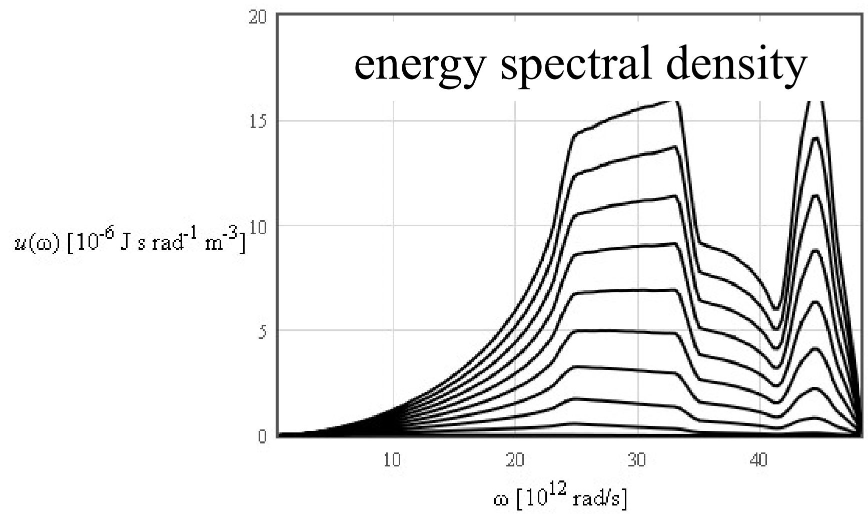




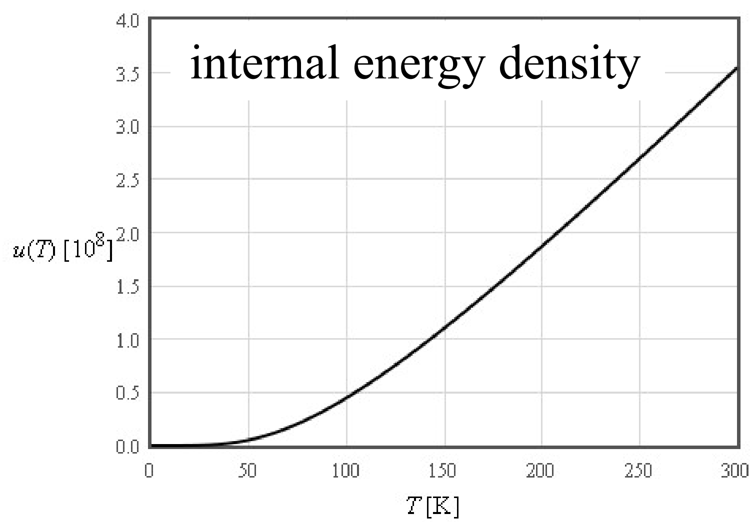
fcc phonons



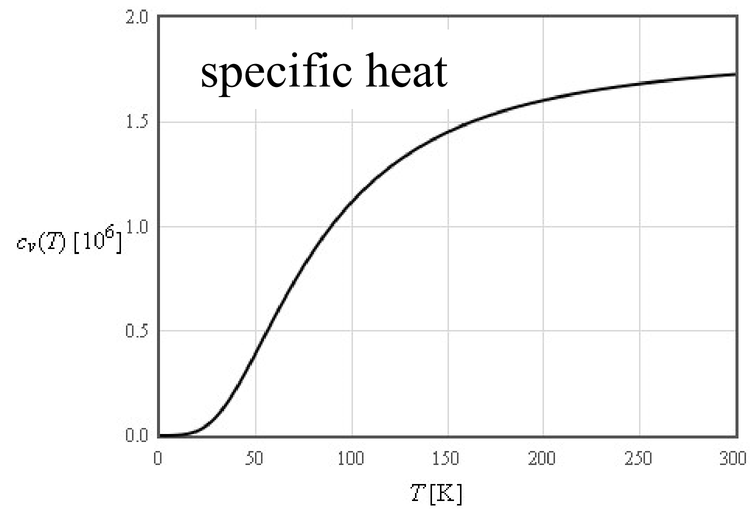
$D(\omega)$ [10^{15} s/m³]
ω [10^{12} Hz]



energy spectral density
$u(\omega)$ [10^{-6} J s rad^{-1} m^{-3}]
ω [10^{12} rad/s]

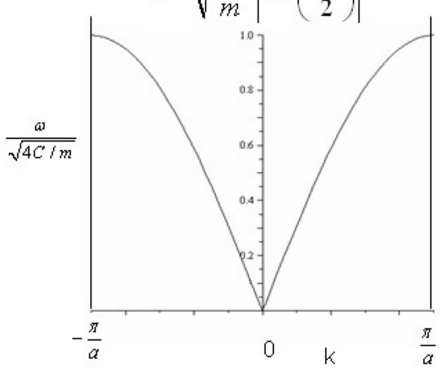
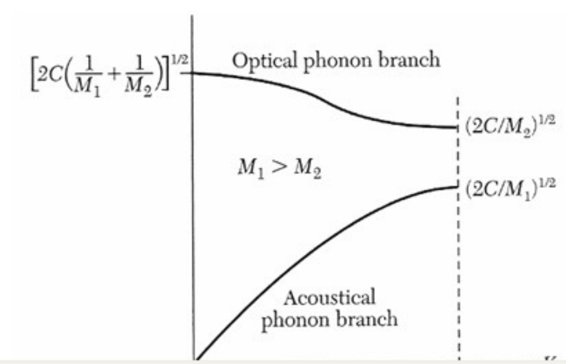


internal energy density
$u(T)$ [10^8]
T [K]

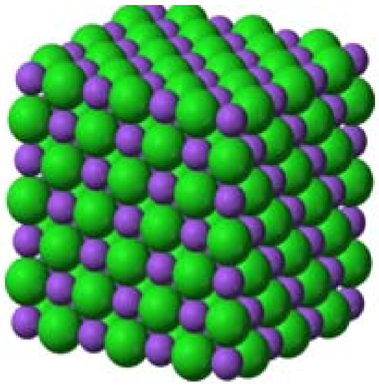


specific heat
$c_V(T)$ [10^6]
T [K]

http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/phonontable.html

	Linear Chain $m\frac{d^2u_s}{dt^2}=C(u_{s+1}-2u_s+u_{s-1})$	**Linear chain 2 masses** $M_1\frac{d^2u_s}{dt^2}=C(v_{s-1}-2u_s+v_s)$ $M_2\frac{d^2v_s}{dt^2}=C(u_s-2v_s+u_{s+1})$	**Linear chain 2 spring constants** $M\frac{d^2u_s}{dt^2}=C_1(v_{s-1}-2u_s+v_s)$ $M\frac{d^2v_s}{dt^2}=C_2(u_s-2v_s+u_{s+1})$	n
Eigenfunction solutions	$u_s=A_k e^{i(ksa-\omega t)}$	$u_s=ue^{i(ksa-\omega t)}$ $v_s=ve^{i(ksa-\omega t)}$	$u_s=ue^{i(ksa-\omega t)}$ $v_s=ve^{i(ksa-\omega t)}$	
Dispersion relation	$\omega=\sqrt{\frac{4C}{m}}\left\lvert\sin\left(\frac{ka}{2}\right)\right\rvert$ 	$\omega^2=C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)\pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2-\frac{4\sin^2 ka}{M_1M_2}}$ 		

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:

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

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

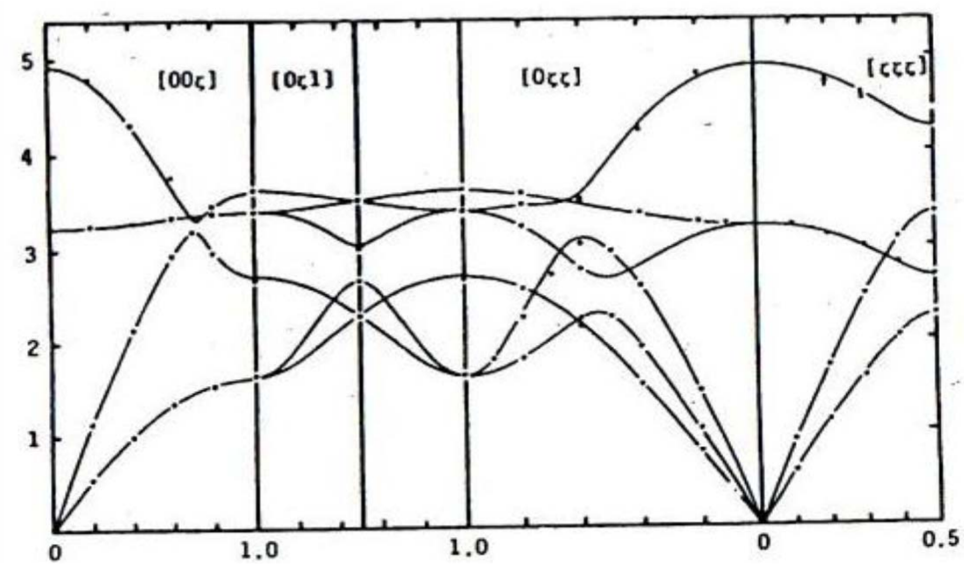
z - Richtung:

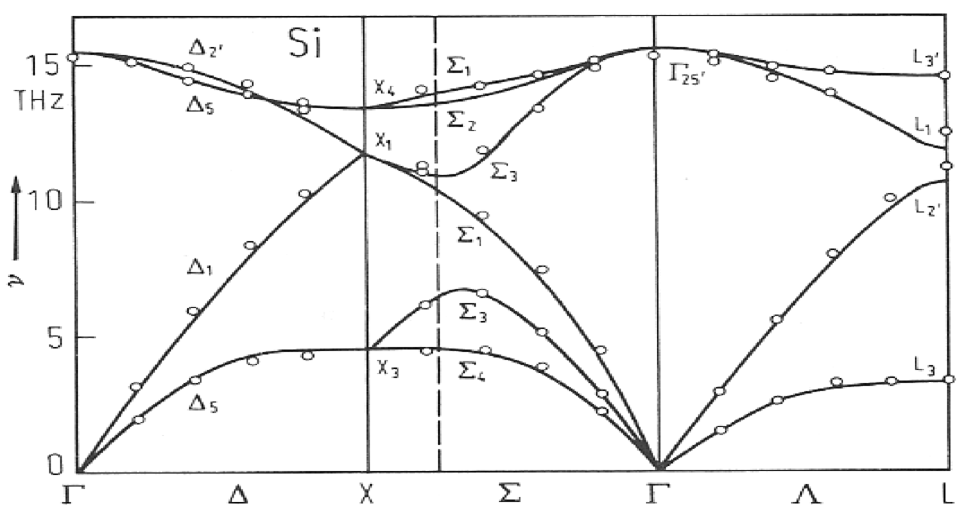
$$M_1 \frac{d^2 u^z_{nml}}{dt^2} = C\left(-2u^z_{nml} + v^z_{n(m-1)(l-1)} + v^z_{(n-1)ml}\right)$$

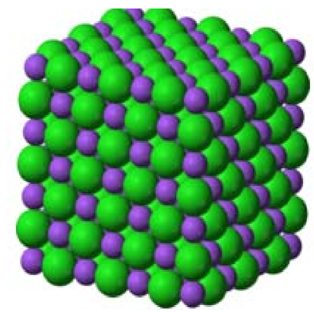
$$M_2 \frac{d^2 v^z_{nml}}{dt^2} = C\left(-2v^z_{nml} + u^z_{n(m+1)(l+1)} + u^z_{(n+1)ml}\right)$$

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

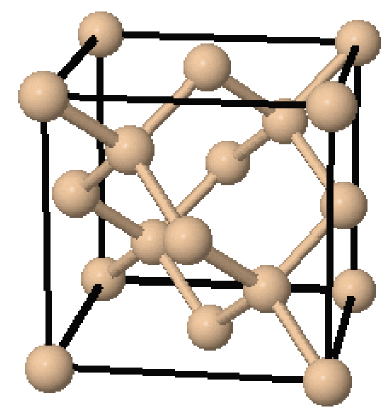
Two atoms per primitive unit cell







NaCl

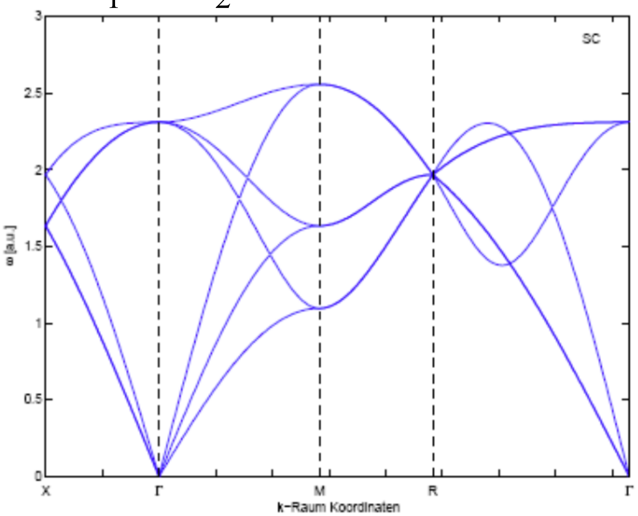


Si

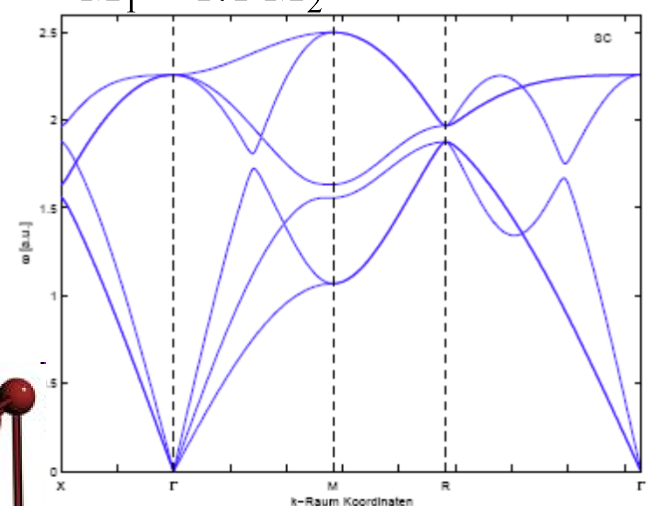
CsCl

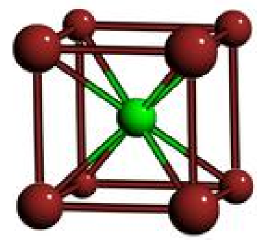
Hannes Brandner

$M_1 = M_2$

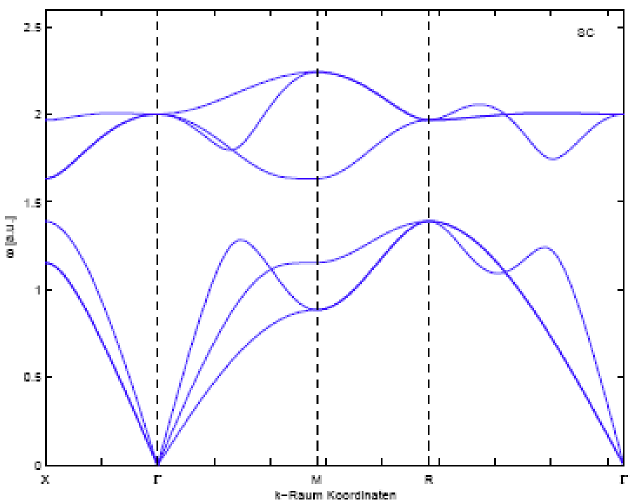


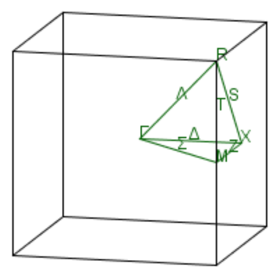
$M_1 = 1.1\ M_2$



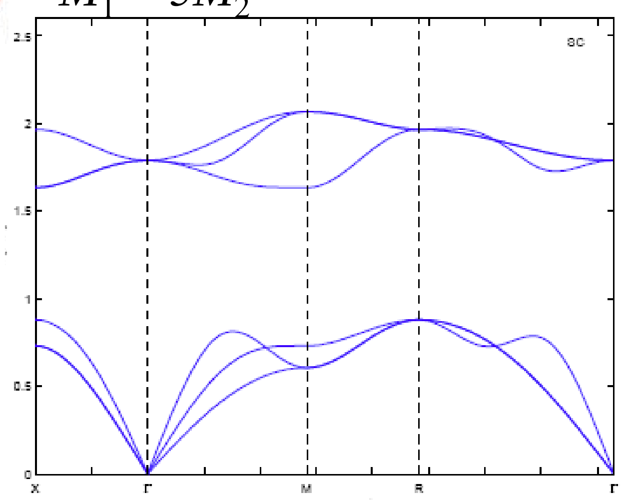


$M_1 = 2M_2$





$M_1 = 5M_2$



GaAs

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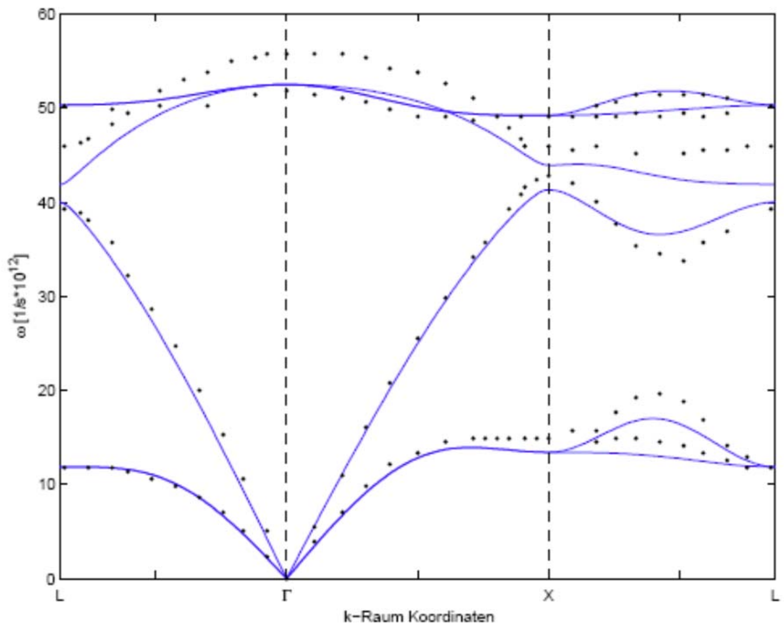
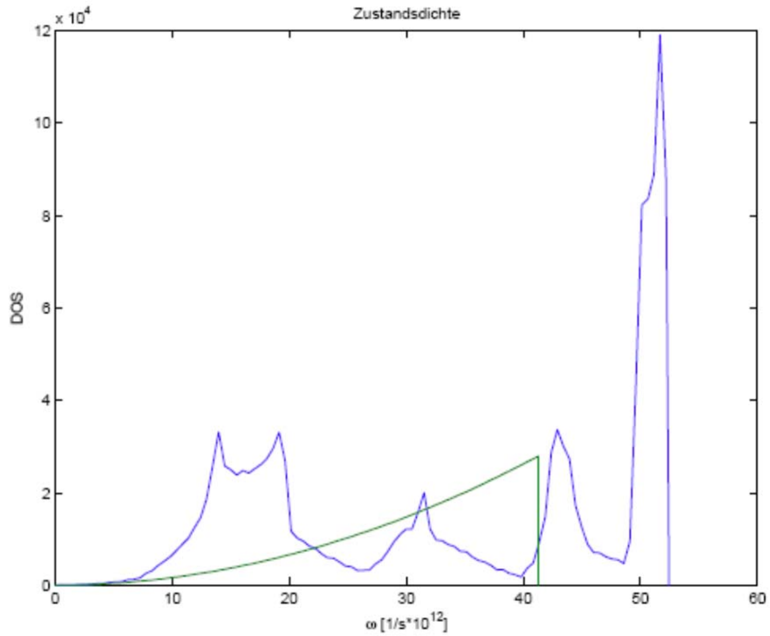
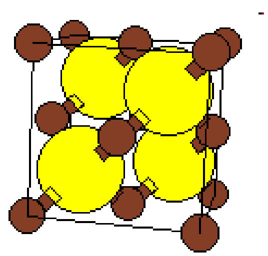
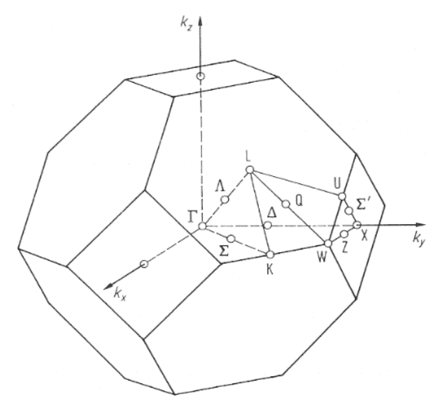








Phonon quasiparticle lifetime

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.

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

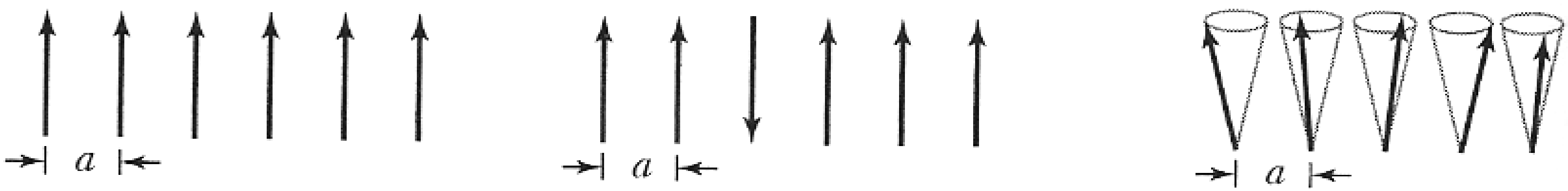
Occupation is determined by a master equation (not the Bose-Einstein function).

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

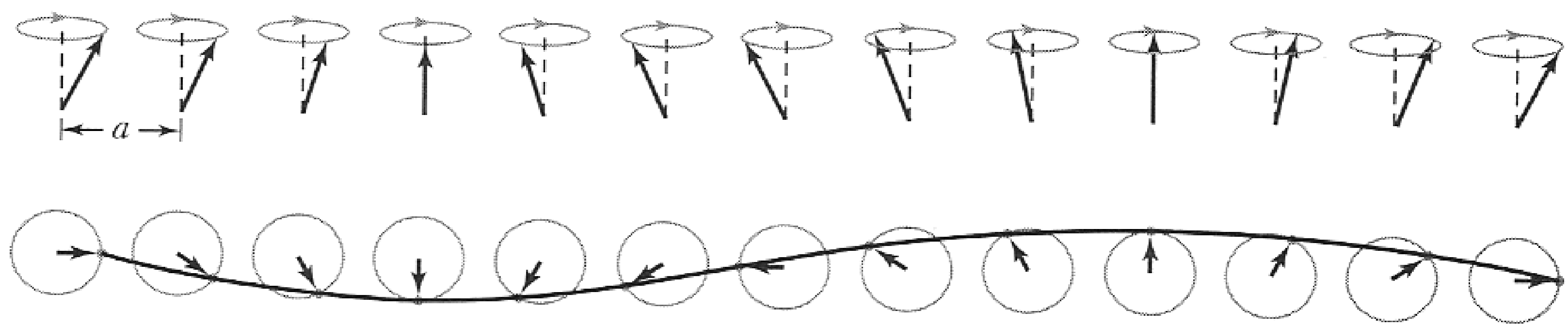
Acoustic attenuation

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.

Magnons



Magnons are excitations of the ordered ferromagnetic state



Magnons

Energy of the Heisenberg term involving spin *p*

$$-2J\vec{S}_p \cdot \left(\vec{S}_{p+1} + \vec{S}_{p-1}\right)$$

The magnetic moment of spin *p* is

$$\vec{\mu}_p = -g\mu_B \vec{S}_p$$

$$-\vec{\mu}_p \cdot \left(\frac{-2J}{g\mu_B}\right)\left(\vec{S}_{p+1} + \vec{S}_{p-1}\right)$$

This has the form $-\mu_p \cdot B_p$ where B_p is

$$\vec{B}_p = \left(\frac{-2J}{g\mu_B}\right)\left(\vec{S}_{p+1} + \vec{S}_{p-1}\right)$$

Magnons

$$\vec{\mu}_p = -g\mu_B \vec{S}_p \qquad \vec{B}_p = \left(\frac{-2J}{g\mu_B}\right)\left(\vec{S}_{p+1} + \vec{S}_{p-1}\right)$$

The rate of change of angular momentum is the torque

$$\hbar \frac{d\vec{S}_p}{dt} = \vec{\mu}_p \times \vec{B}_p = 2J\left(\vec{S}_p \times \vec{S}_{p+1} + \vec{S}_p \times \vec{S}_{p-1}\right)$$

If the amplitude of the deviations from perfect alignment along the z-axis are small:

$$\hbar \frac{dS_p^x}{dt} = 2J\left|S\right|\left(S_{p+1}^y - 2S_p^y + S_{p-1}^y\right)$$

$$\hbar \frac{dS_p^y}{dt} = 2J\left|S\right|\left(S_{p+1}^x - 2S_p^x + S_{p-1}^x\right)$$

$$\hbar \frac{d\vec{S}_p^z}{dt} = 0$$

Magnons

$$\hbar \frac{dS_p^x}{dt} = 2J\left|S\right|\left(S_{p+1}^y - 2S_p^y + S_{p-1}^y\right)$$

$$\hbar \frac{dS_p^y}{dt} = 2J\left|S\right|\left(S_{p+1}^x - 2S_p^x + S_{p-1}^x\right)$$

$$\hbar \frac{dS_p^z}{dt} = 0$$

These are coupled linear differential equations. The solutions have the form:

$$\begin{pmatrix} S_p^x \\ S_p^y \end{pmatrix} = \begin{pmatrix} u_k^x \\ u_k^y \end{pmatrix} \exp\left[i\left(kpa - \omega t\right)\right]$$

$$-i\hbar\omega u_k^x e^{ikpa} = 2J\left|S\right|\left(-e^{ik(p+1)a} + 2e^{ikpa} - e^{-ik(p-1)a}\right)u_k^y$$

$$-i\hbar\omega u_k^y e^{ikpa} = -2J\left|S\right|\left(-e^{ik(p+1)a} + 2e^{ikpa} - e^{-ik(p-1)a}\right)u_k^x$$

Cancel a factor of e^{ikpa}.

Magnons

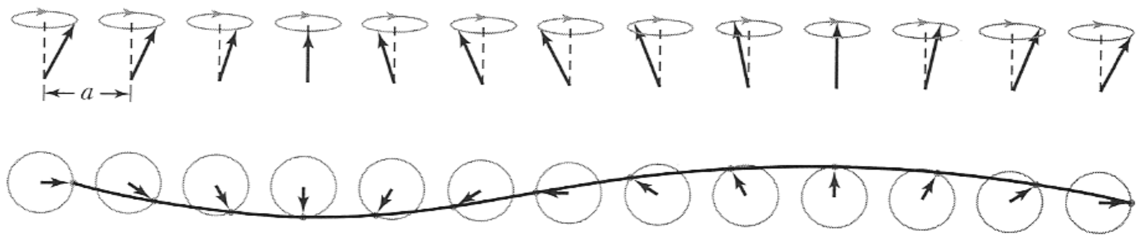
$$-i\hbar\omega u_k^x = 2J\left|S\right|\left(-e^{ika} + 2 - e^{-ika}\right)u_k^y$$
$$-i\hbar\omega u_k^y = -2J\left|S\right|\left(-e^{ika} + 2 - e^{-ika}\right)u_k^x$$

These equations will have solutions when,

$$\begin{vmatrix} i\hbar\omega & 4J\left|S\right|\left(1-\cos(ka)\right) \\ -4J\left|S\right|\left(1-\cos(ka)\right) & i\hbar\omega \end{vmatrix} = 0$$

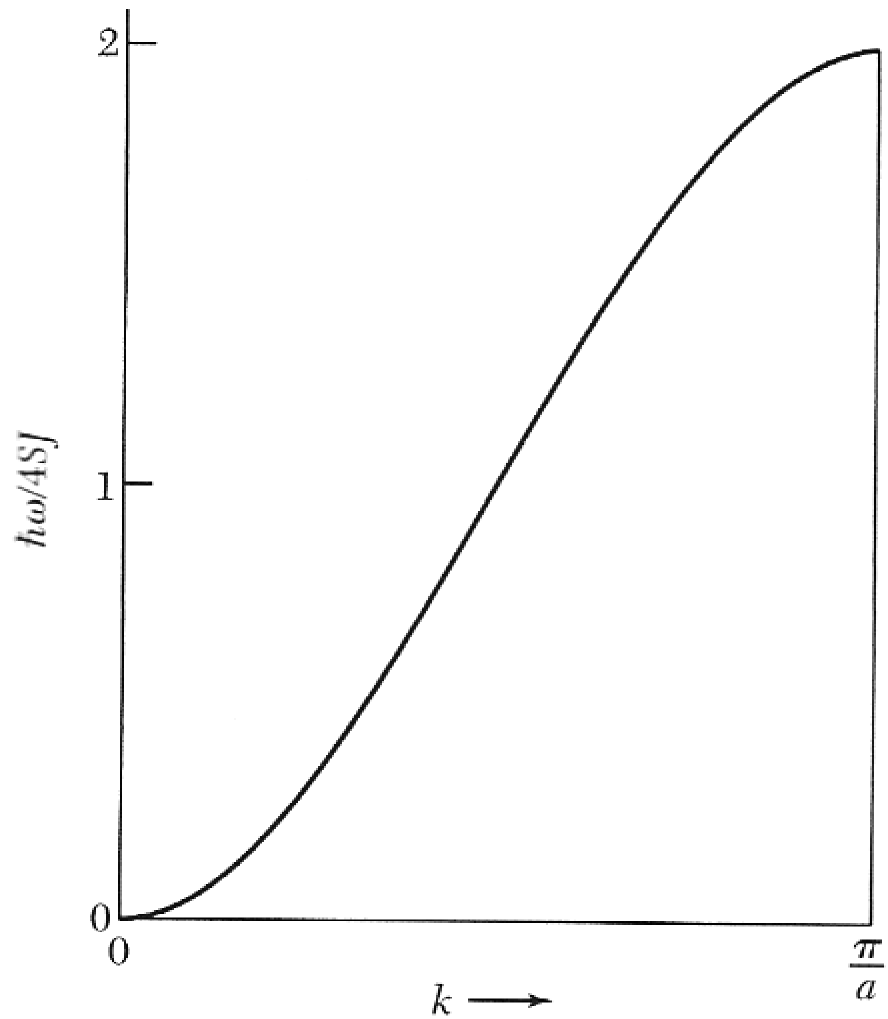
The dispersion relation is:

$$\hbar\omega = 4J\left|S\right|\left(1-\cos(ka)\right)$$



Magnon dispersion relation

$$\hbar\omega = 4JS\left(1 - \cos(ka)\right)$$

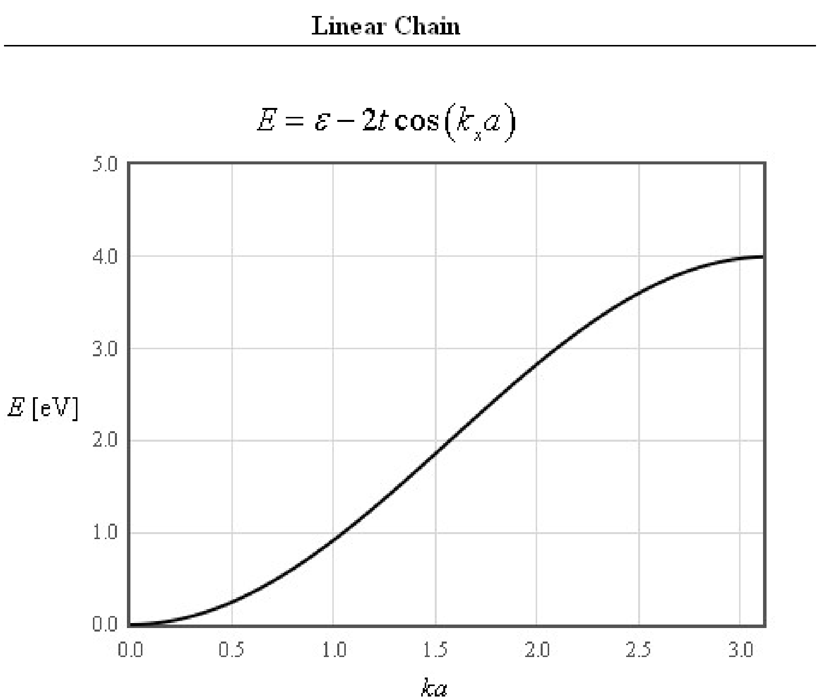


A phonon dispersion relation would be linear at the origin

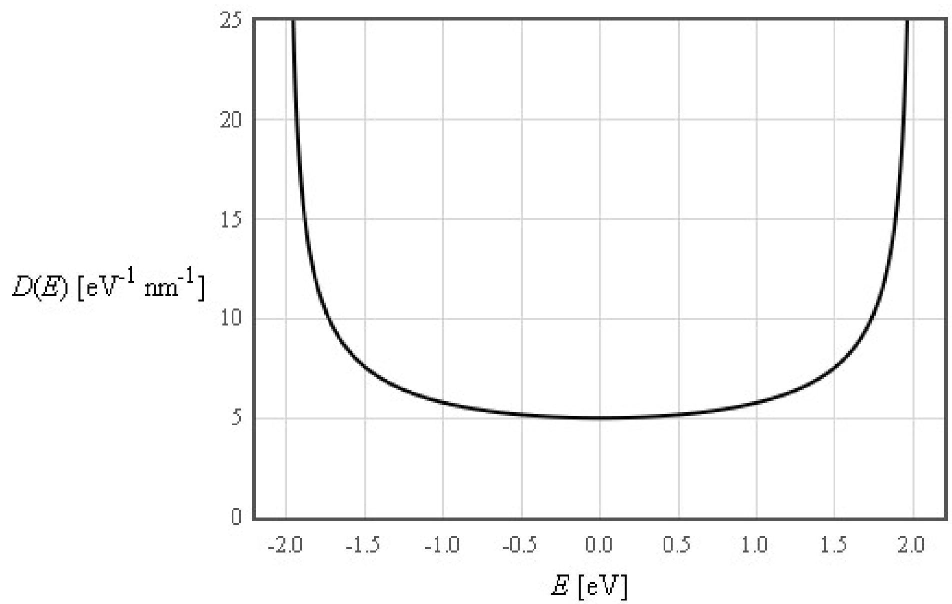
Magnon density of states

$$\hbar\omega = 4JS\left(1-\cos(ka)\right)$$

Mathematically this is the same problem as the tight binding model for electrons on a one-dimensional chain.



$$D(E) = \frac{1}{at\sqrt{1-\left(\frac{\varepsilon - E}{2t}\right)^2}} \quad \mathrm{J^{-1}m^{-1}}$$



Density of states → Specific heat

The specific heat is the derivative of the internal energy with respect to the temperature.

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

This can be expressed in terms of an integral over the frequency ω.

$$c_v = \frac{\partial}{\partial T}\int u(\omega)d\omega = \frac{\partial}{\partial T}\int \hbar\omega D(\omega)\frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1}d\omega$$

The Leibniz integral rule can be used to bring the differentiation inside the integral. If the phonon density of states $D(\omega)$ is temperature independent, the result is,

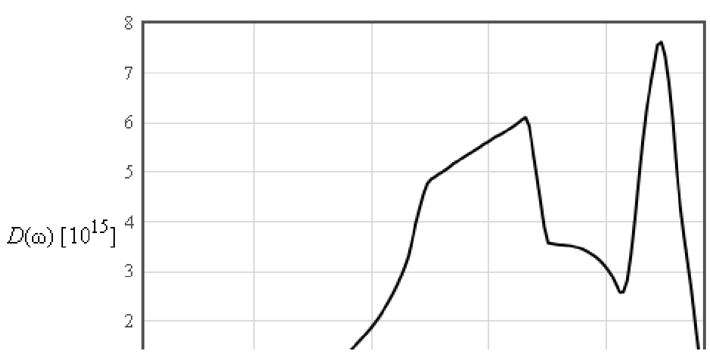
$$c_v = \int \hbar\omega D(\omega)\frac{\partial}{\partial T}\left(\frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1}\right)d\omega$$

Since only the Bose-Einstein factor depends on temperature, the differentiation can be performed analytically and the expression for the specific heat is,

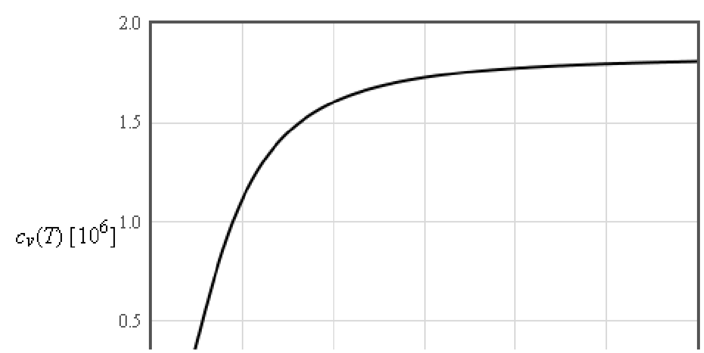
$$c_v = \int \left(\frac{\hbar\omega}{T}\right)^2 \frac{D(\omega)e^{\frac{\hbar\omega}{k_BT}}}{k_B\cdot\left(e^{\frac{\hbar\omega}{k_BT}}-1\right)^2}d\omega$$

The form below uses this formula to calculate the temperature dependence of the specific heat from tabulated data for the density of states. The density of states data is input as two columns in the textbox at the lower left. The first column is the angular-frequency ω in rad/s. The second column is the density of states. The units of the density of states depends on the dimensionality: s/m for 1d, s/m^2 for 2d, and s/m^3 for 3d.

After the 'DoS → cv(T)' button is pressed, the density of states is plotted on the left and $c_V(T)$ is plotted from temperature T_{min} to temperature T_{max} on the right. The data for the $c_V(T)$ plot also appear in tabular form in the lower right textbox. The first column is the temperature in Kelvin and the second column is the specific heat in units of J K^{-1} m^{-1}, J K^{-1} m^{-3}, or J K^{-1} m^{-3} depending on the dimensionality.



DoS → cv(T)



Ferromagnetic magnons - simple cubic

The dispersion relation in one dimension:

$$\hbar\omega = 4J\left|S\right|\left(1-\cos(ka)\right)$$

The dispersion relation for a cubic lattice in three dimensions:

$$\hbar\omega = 2J\left|S\right|\left(z-\sum_{\vec{\delta}}\cos(\vec{k}\cdot\vec{\delta})\right)$$

The magnon contribution to thermodynamic properties can be calculated similar to the phonon contribution to the thermodynamic properties.