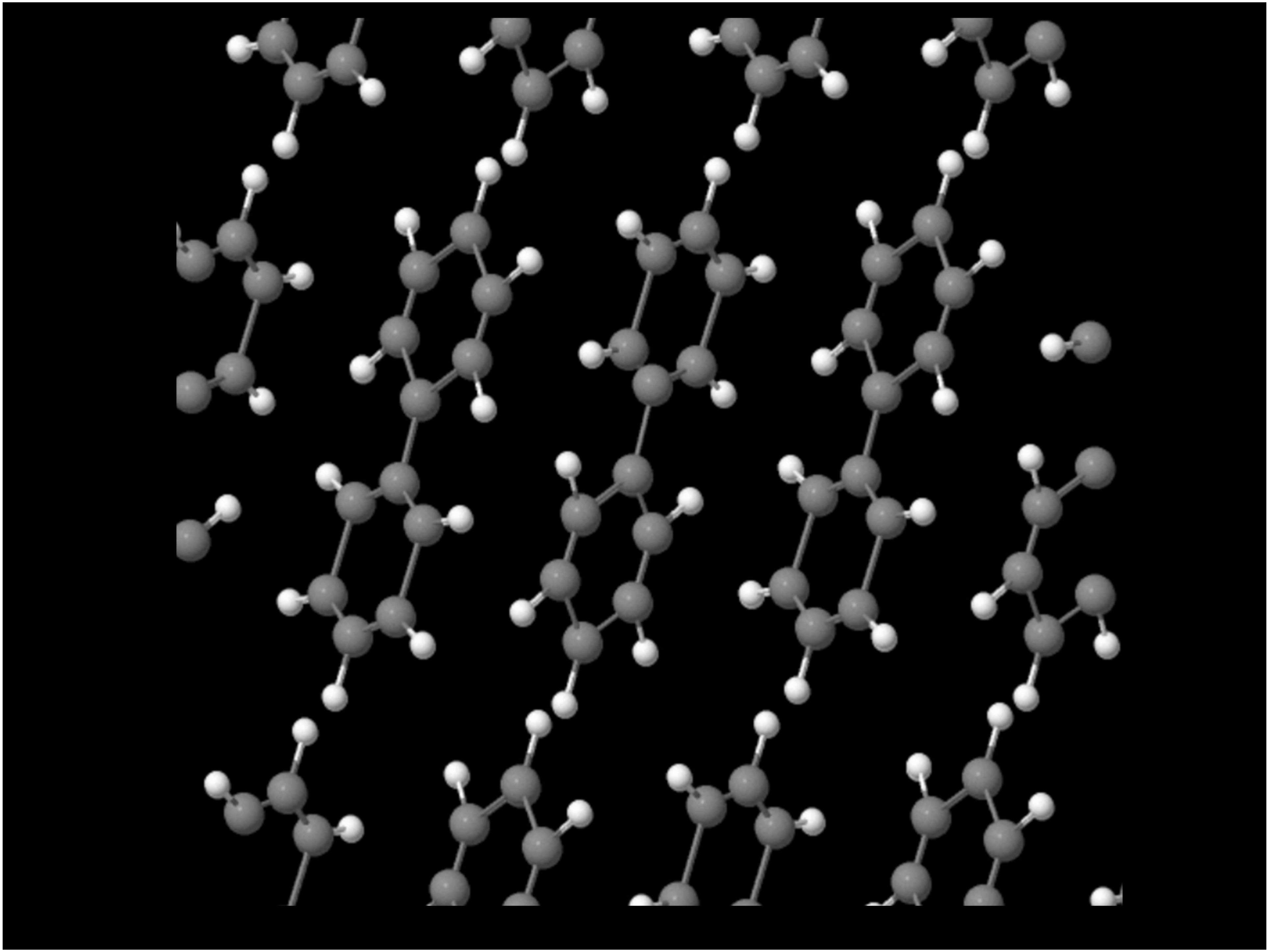
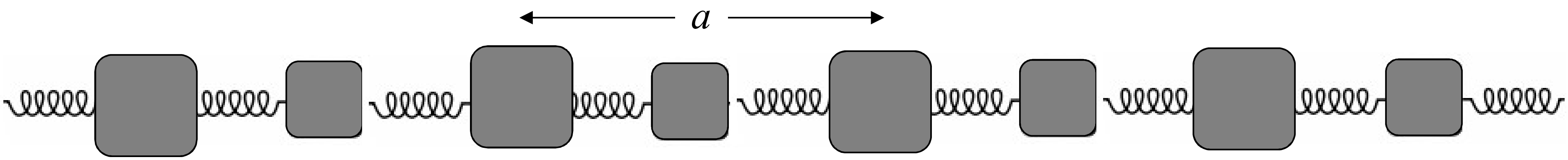
# Phonons



# Linear chain $M_1$ and $M_2$




Newton's law:

$$M_1 \frac{d^2 u_s}{dt^2} = C(v_{s-1} - 2u_s + v_s)$$

$2N$ modes

$$M_2 \frac{d^2 v_s}{dt^2} = C(u_s - 2v_s + u_{s+1})$$

assume harmonic solutions

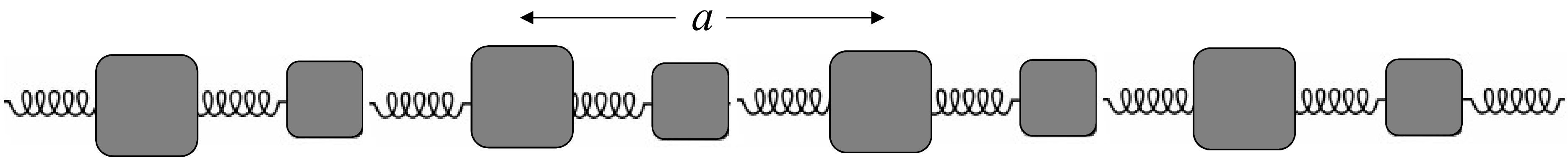
$$u_s = u_k e^{i(ksa - \omega t)}$$

$$v_s = v_k e^{i(ksa - \omega t)}$$

$$-\omega^2 M_1 u_k = C v_k (1 + \exp(-ika)) - 2C u_k$$

$$-\omega^2 M_2 v_k = C u_k (1 + \exp(ika)) - 2C v_k$$

# Linear chain $M_1$ and $M_2$



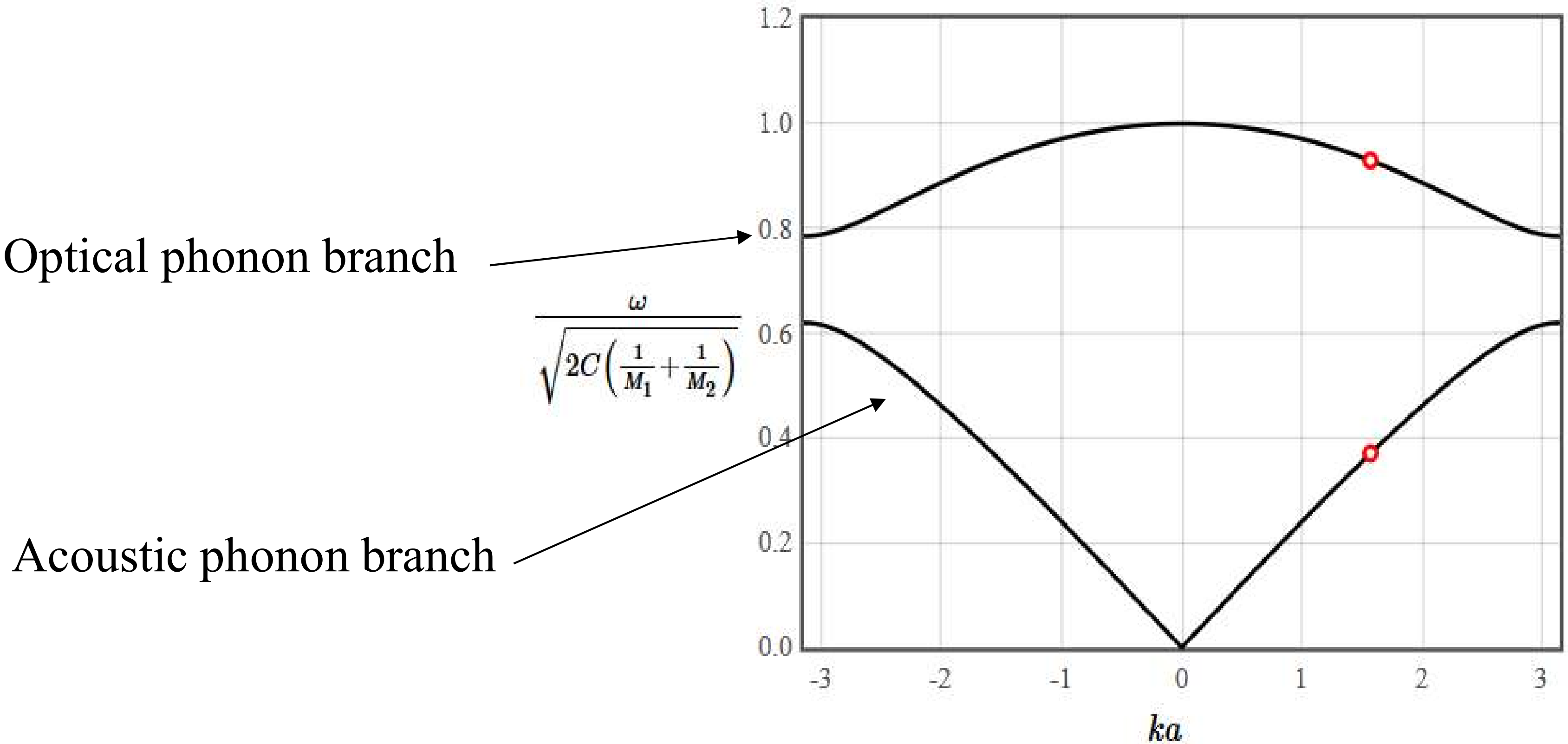

$$-\omega^2 M_1 u_k = C v_k (1+\exp(-ika)) - 2Cu_k$$
$$-\omega^2 M_2 v_k = C u_k (1+\exp(ika)) - 2Cv_k$$

$$\begin{bmatrix} \omega^2 M_1 - 2C & C(1+\exp(-ika)) \\ C(1+\exp(ika)) & \omega^2 M_2 - 2C \end{bmatrix} \begin{bmatrix} u_k \\ v_k \end{bmatrix} = 0$$

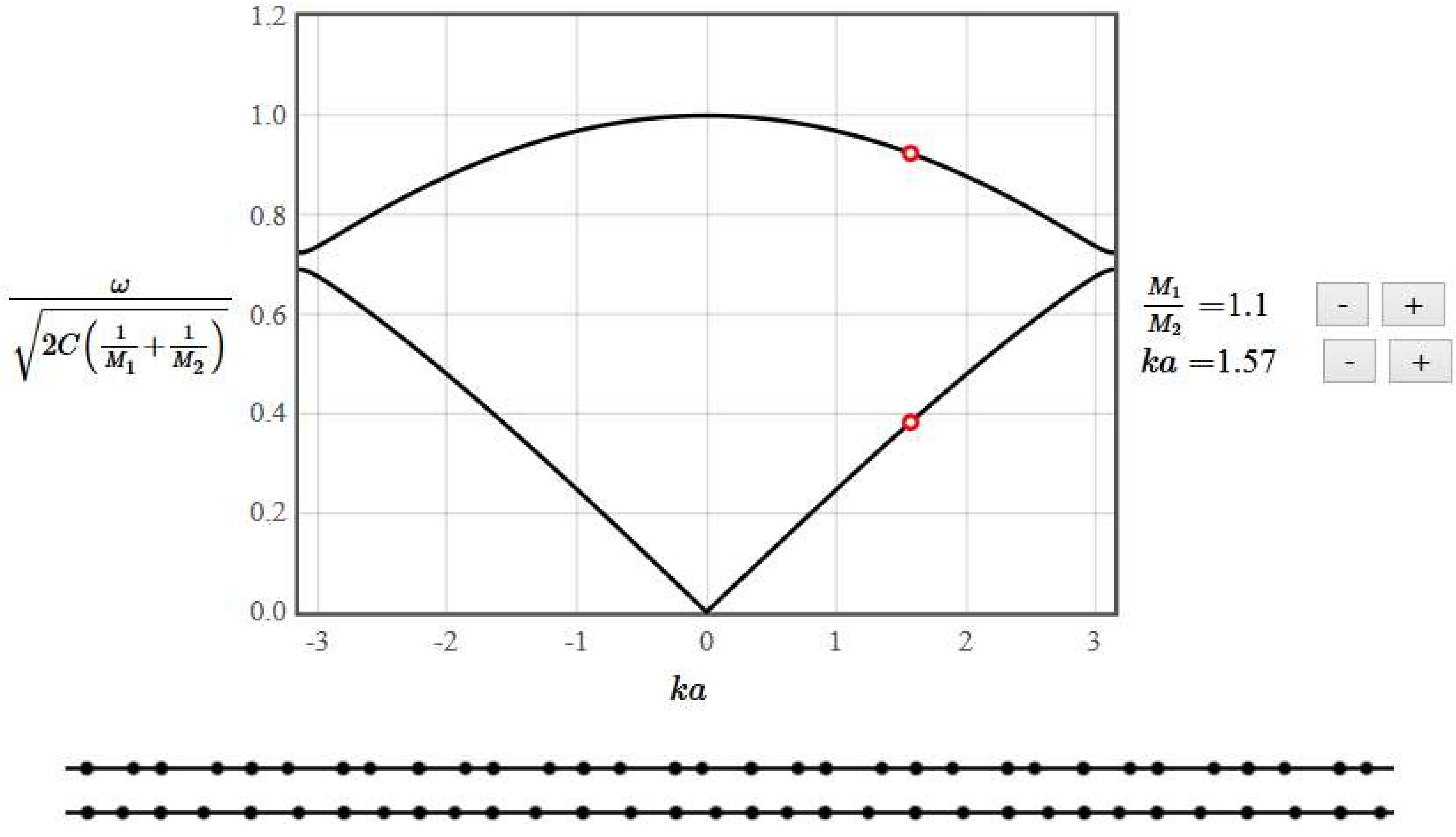
$$M_1 M_2 \omega^4 - 2C\left(M_1 + M_2\right)\omega^2 + 2C^2\left(1-\cos(ka)\right) = 0$$

# dispersion relation

$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2\left(\frac{ka}{2}\right)}{M_1M_2}}$$

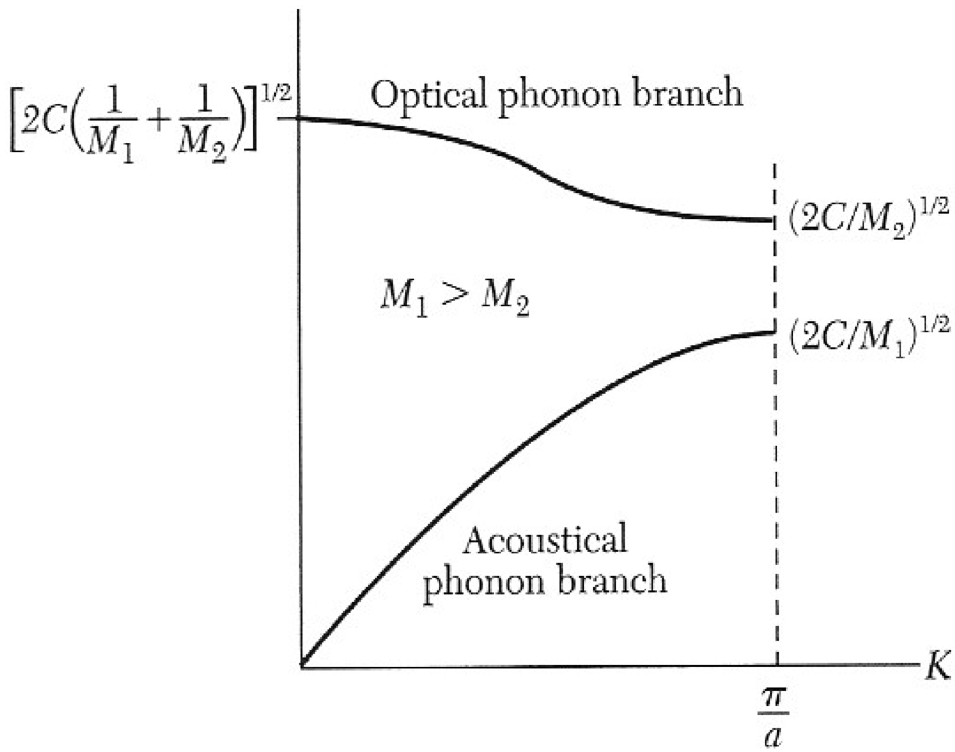


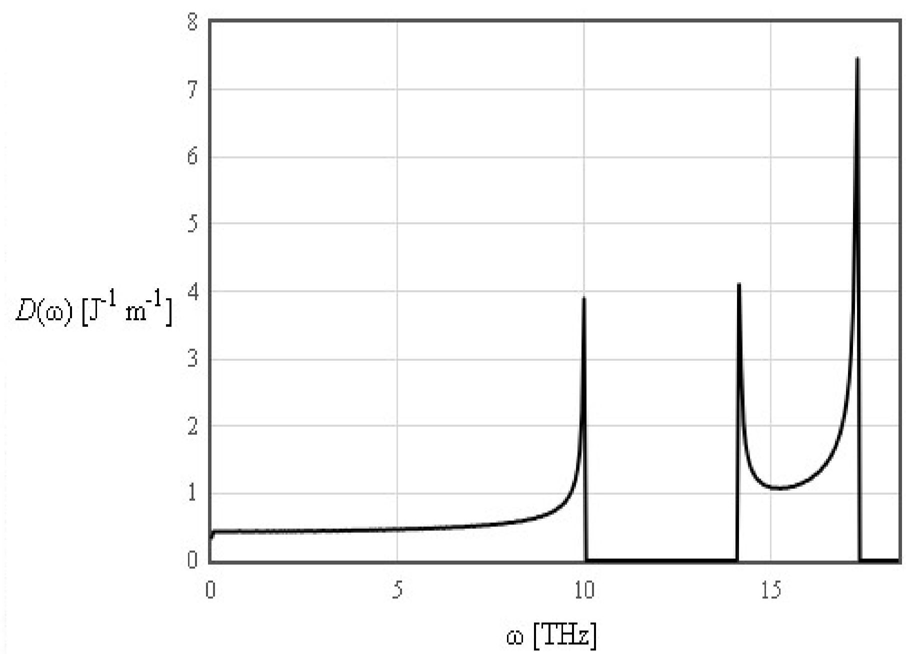
# normal modes




http://lampx.tugraz.at/~hadley/ss1/phonons/1d/1d2m.php

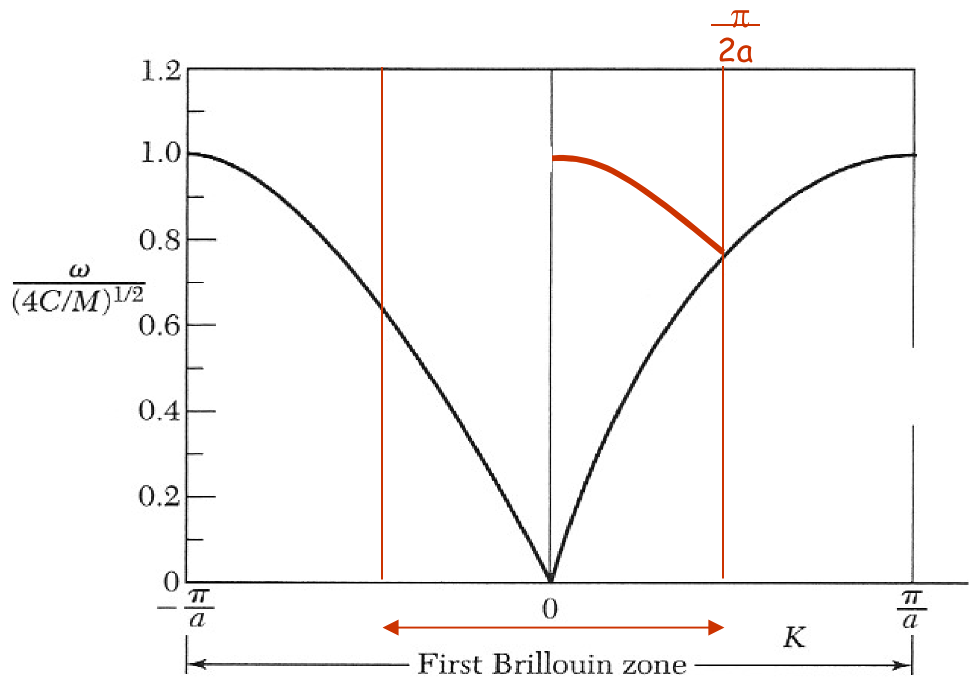
# density of states

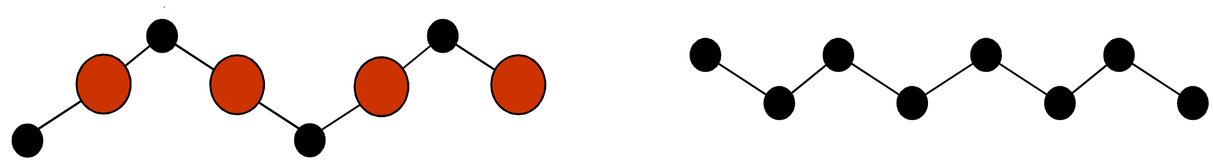



$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2 ka}{M_1 M_2}}$$

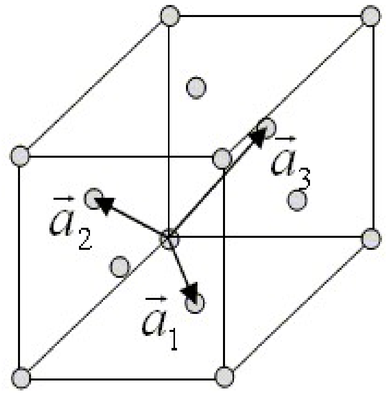
# Linear chain $M_1$ and $M_2$



The branches of the dispersion curves can be translated by a reciprocal lattice vector $\vec{G}$.

# fcc




$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} \qquad \vec{b}_1 = \frac{2\pi}{a}\left(\hat{k}_x + \hat{k}_y - \hat{k}_z\right)$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z} \qquad \vec{b}_2 = \frac{2\pi}{a}\left(\hat{k}_x - \hat{k}_y + \hat{k}_z\right)$$

$$\vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z} \qquad \vec{b}_3 = \frac{2\pi}{a}\left(-\hat{k}_x + \hat{k}_y + \hat{k}_z\right)$$

$$m\frac{d^2u_{lmn}^x}{dt^2} = \frac{C}{2}\Big[\left(u_{l+1mn}^x - u_{lmn}^x\right) + \left(u_{l-1mn}^x - u_{lmn}^x\right) + \left(u_{lm+1n}^x - u_{lmn}^x\right) + \left(u_{lm-1n}^x - u_{lmn}^x\right)$$
$$+\left(u_{l+1mn-1}^x - u_{lmn}^x\right) + \left(u_{l-1mn+1}^x - u_{lmn}^x\right) + \left(u_{lm+1n-1}^x - u_{lmn}^x\right) + \left(u_{lm-1n+1}^x - u_{lmn}^x\right)$$
$$+\left(u_{l+1mn}^y - u_{lmn}^y\right) + \left(u_{l-1mn}^y - u_{lmn}^y\right) - \left(u_{lm+1n-1}^y - u_{lmn}^y\right) - \left(u_{lm-1n+1}^y - u_{lmn}^y\right)$$
$$+\left(u_{lm+1n}^z - u_{lmn}^z\right) + \left(u_{lm-1n}^z - u_{lmn}^z\right) - \left(u_{l+1mn-1}^z - u_{lmn}^z\right) - \left(u_{l-1mn+1}^z - u_{lmn}^z\right)\Big]$$

and similar expressions for the $y$ and $z$ motion

# Normal modes are eigenfunctions of T

$$u^x_{lmn} = u^x_{\vec{k}} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

$$u^y_{lmn} = u^y_{\vec{k}} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

$$u^z_{lmn} = u^z_{\vec{k}} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

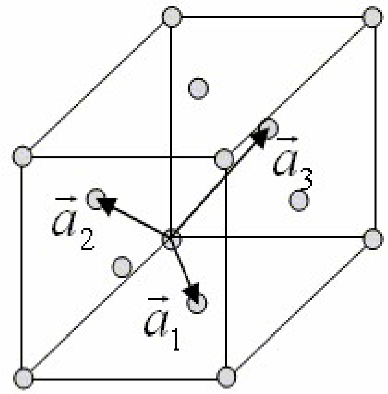
These are eigenfunctions of T.

$$T_{pqr}u^x_{lmn} = u^x_{\vec{k}} \exp\left(i\left(l\vec{k}\cdot\left(\vec{a}_1 + p\vec{a}_1\right) + m\vec{k}\cdot\left(\vec{a}_2 + q\vec{a}_2\right) + n\vec{k}\cdot\left(\vec{a}_3 + r\vec{a}_3\right) - \omega t\right)\right)$$

$$= \exp\left(i\left(lp\vec{k}\cdot\vec{a}_1 + qm\vec{k}\cdot\vec{a}_2 + rn\vec{k}\cdot\vec{a}_3\right)\right) u^x_{\vec{k}} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

$$= \exp\left(i\left(lp\vec{k}\cdot\vec{a}_1 + qm\vec{k}\cdot\vec{a}_2 + rn\vec{k}\cdot\vec{a}_3\right)\right) u^x_{lmn}$$

# fcc




$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

$$\vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

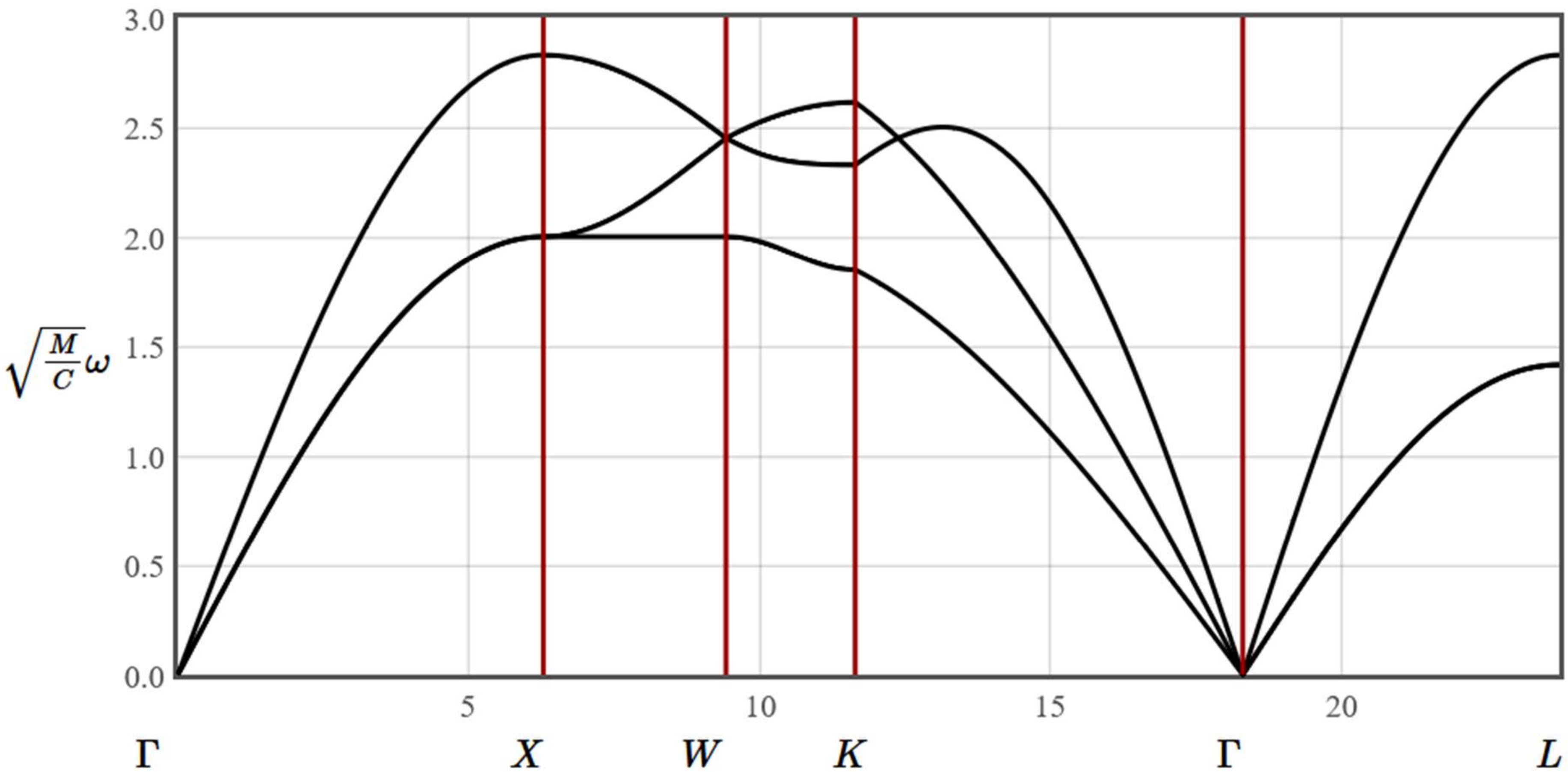
Substitute the eigenfunctions of *T* into Newton's laws.

$$u^x_{lmn} = u^x_{\vec{k}} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3\right)\right) = u^x_{\vec{k}} \exp\left(i\left(\frac{(l+m)k_x a}{2} + \frac{(l+n)k_y a}{2} + \frac{(m+n)k_z a}{2}\right)\right).$$

$$\begin{vmatrix}
4-\cos\left(\frac{k_xa}{2}+\frac{k_ya}{2}\right)-\cos\left(\frac{k_xa}{2}+\frac{k_za}{2}\right)-\cos\left(\frac{k_xa}{2}-\frac{k_ya}{2}\right)-\cos\left(\frac{k_xa}{2}-\frac{k_za}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_xa}{2}+\frac{k_ya}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_ya}{2}\right) & -\cos\left(\frac{k_xa}{2}+\frac{k_za}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_za}{2}\right) \\
-\cos\left(\frac{k_xa}{2}+\frac{k_ya}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_ya}{2}\right) & 4-\cos\left(\frac{k_ya}{2}+\frac{k_xa}{2}\right)-\cos\left(\frac{k_ya}{2}+\frac{k_za}{2}\right)-\cos\left(\frac{k_ya}{2}-\frac{k_xa}{2}\right)-\cos\left(\frac{k_ya}{2}-\frac{k_za}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_ya}{2}+\frac{k_za}{2}\right)+\cos\left(\frac{k_ya}{2}-\frac{k_za}{2}\right) \\
-\cos\left(\frac{k_xa}{2}+\frac{k_za}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_za}{2}\right) & -\cos\left(\frac{k_ya}{2}+\frac{k_za}{2}\right)+\cos\left(\frac{k_ya}{2}-\frac{k_za}{2}\right) & 4-\cos\left(\frac{k_za}{2}+\frac{k_xa}{2}\right)-\cos\left(\frac{k_za}{2}+\frac{k_ya}{2}\right)-\cos\left(\frac{k_za}{2}-\frac{k_xa}{2}\right)-\cos\left(\frac{k_za}{2}-\frac{k_ya}{2}\right)-\frac{m\omega^2}{\sqrt{2}C}
\end{vmatrix} = 0$$

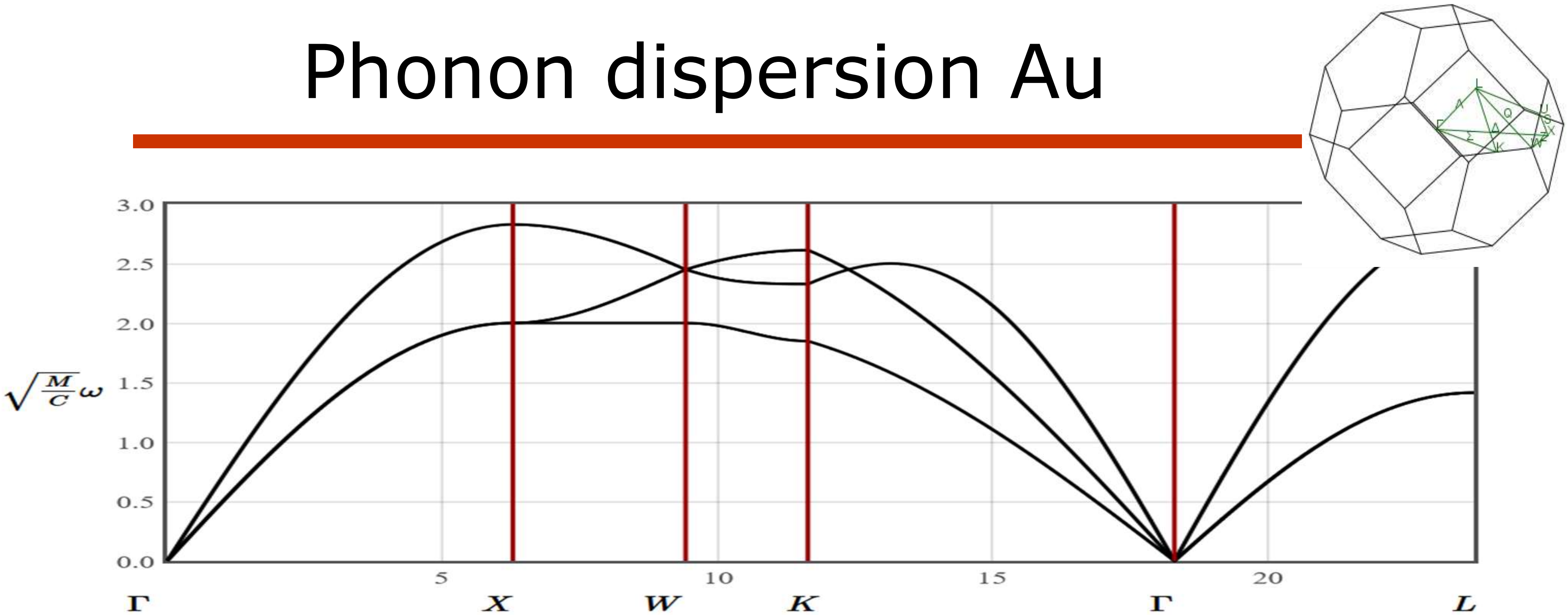
http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/fcc/fcc.html

For every *k* there are 3 solutions for ω.



# Phonon dispersion Au

From Springer Materials: Landholt Boernstein Database



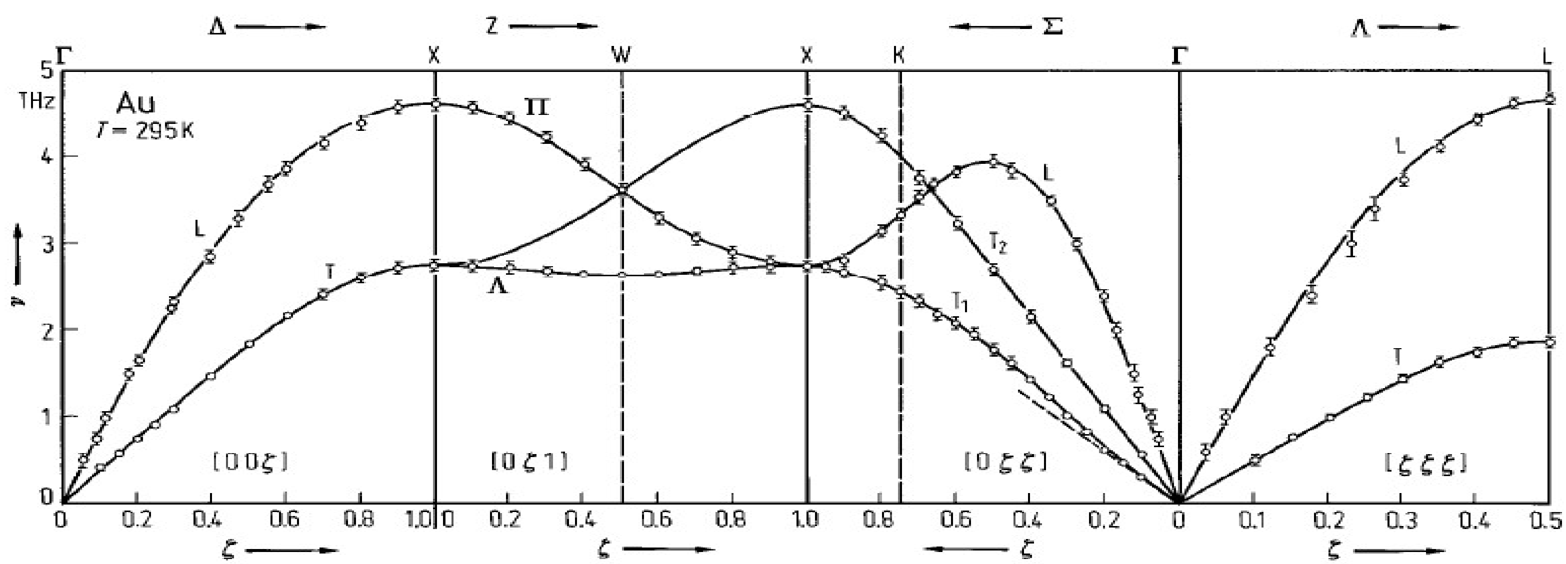
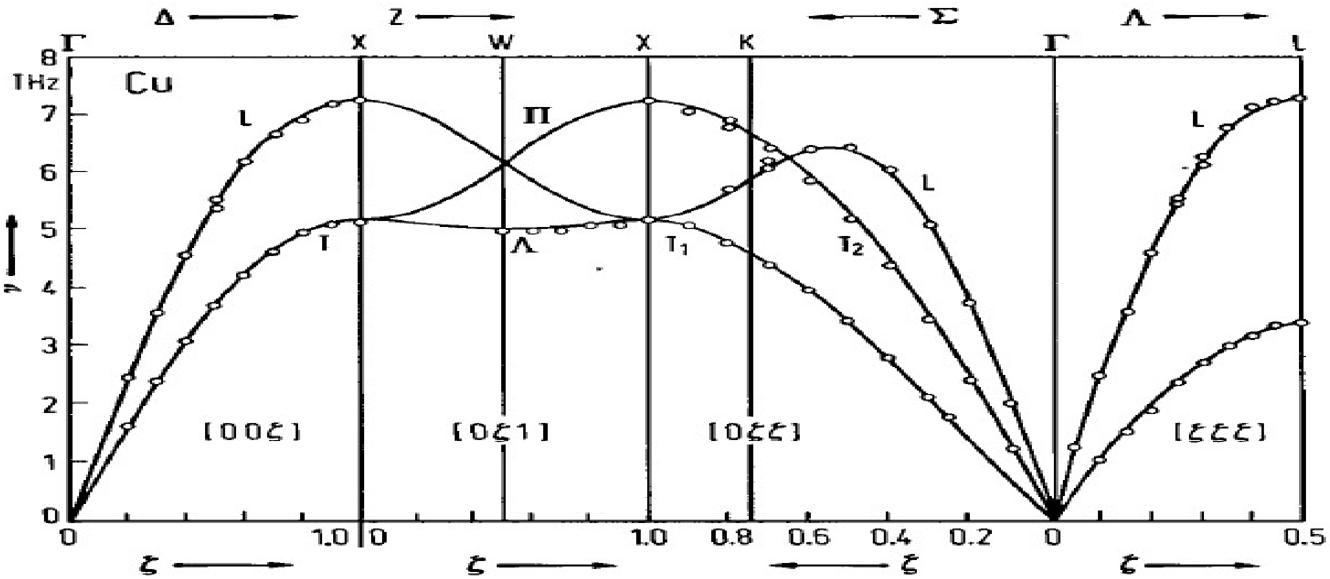
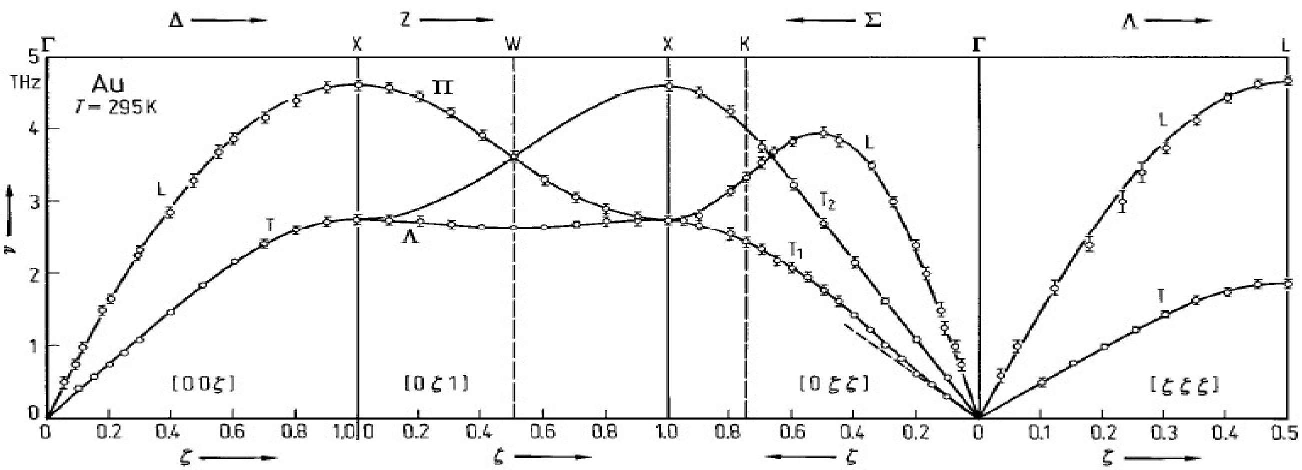




Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the velocity of sound appropriate to the [0ζζ] $T_1$ branch.

# Materials with the same crystal structure will have similar phonon dispersion relations



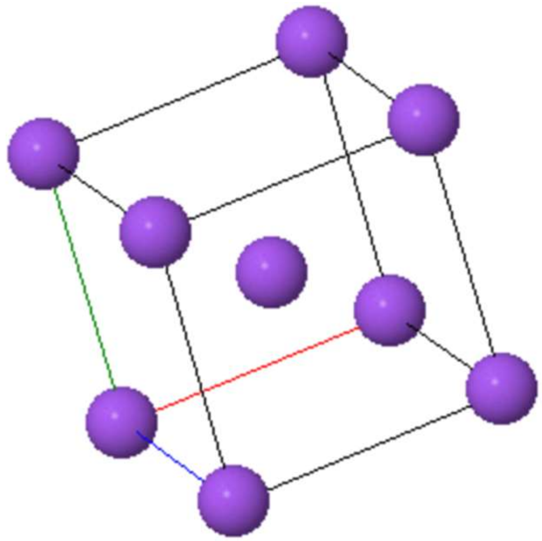

Cu

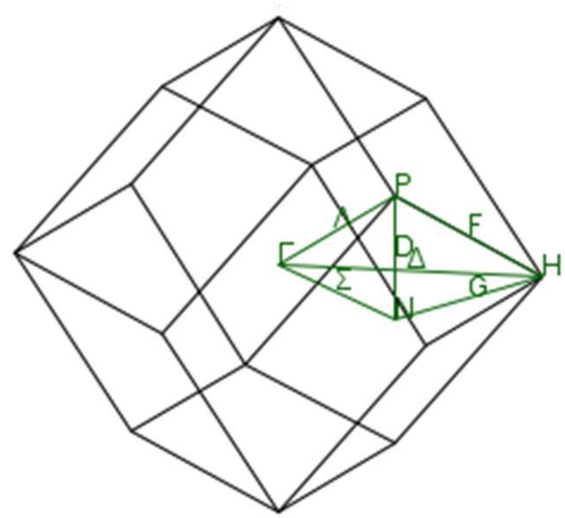


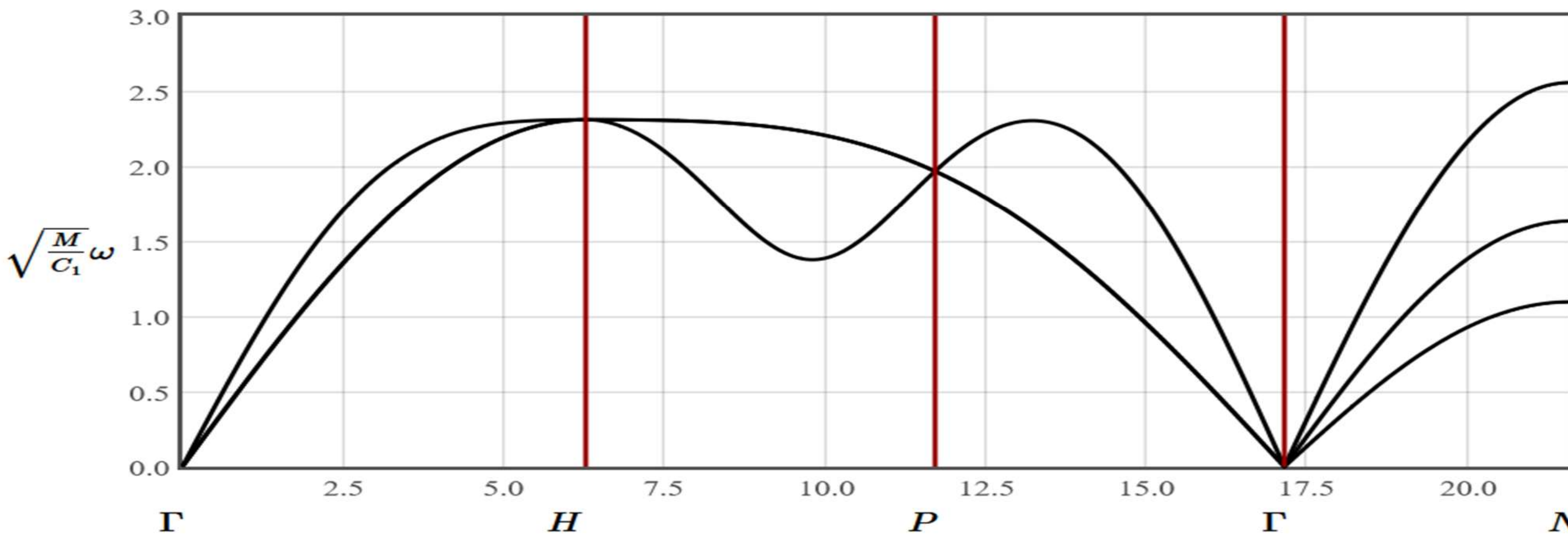

Au

Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the velocity of sound appropriate to the [0ζζ] $T_1$ branch.

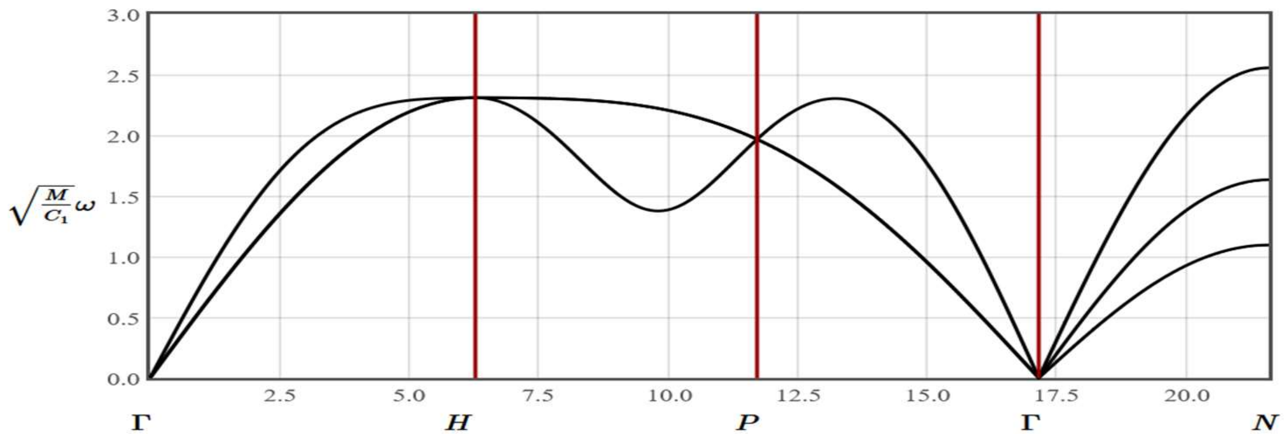
# Phonon dispersion bcc

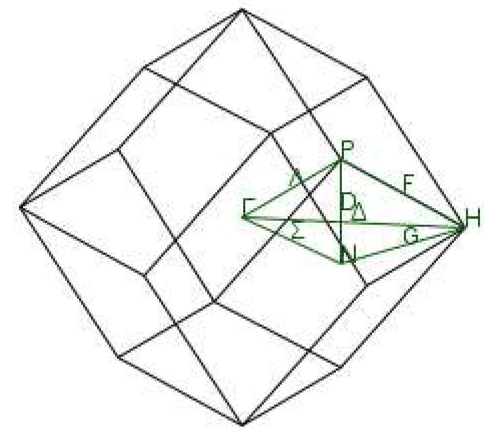




# Phonon dispersion Fe



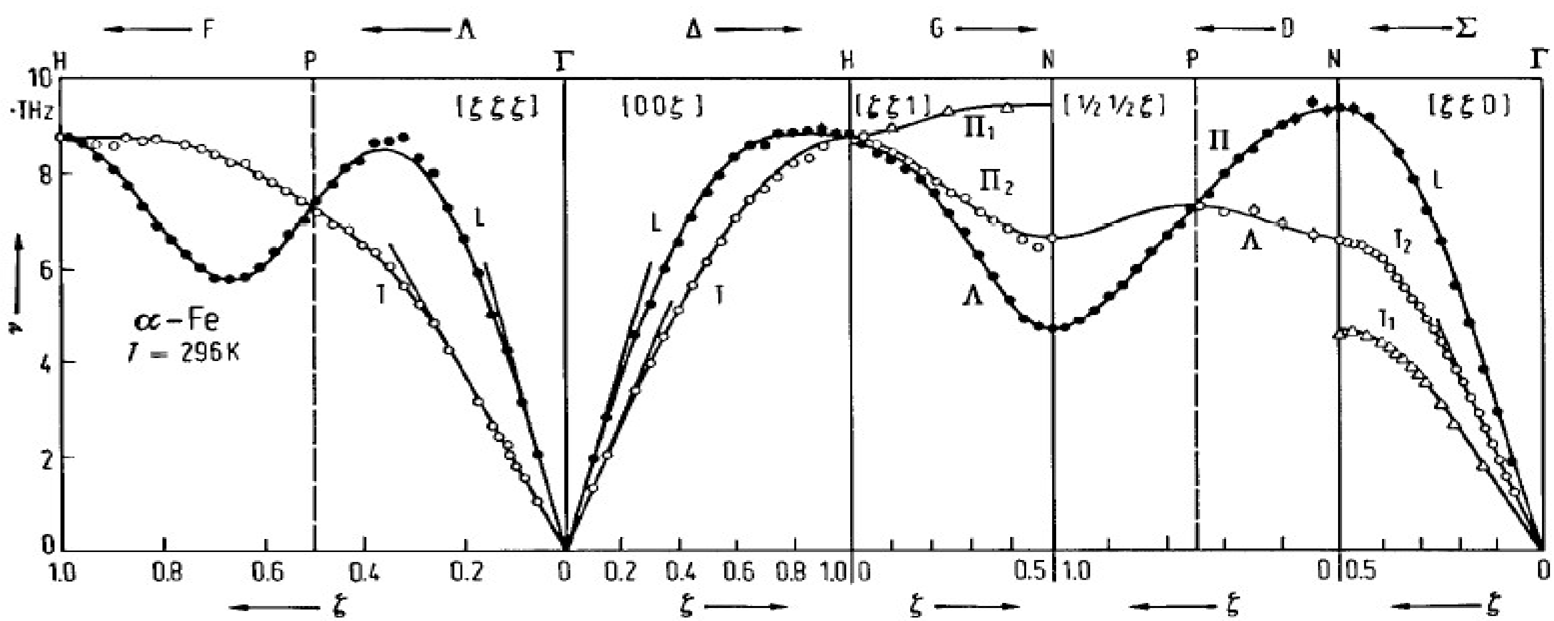




Fig. 2. Fe. Phonon dispersion curves in α-iron at 296 K. Experimental points: [68Va2]. Solid curve: fifth neighbour Born-von Karman model (Table 3 Fe [68Va2]).

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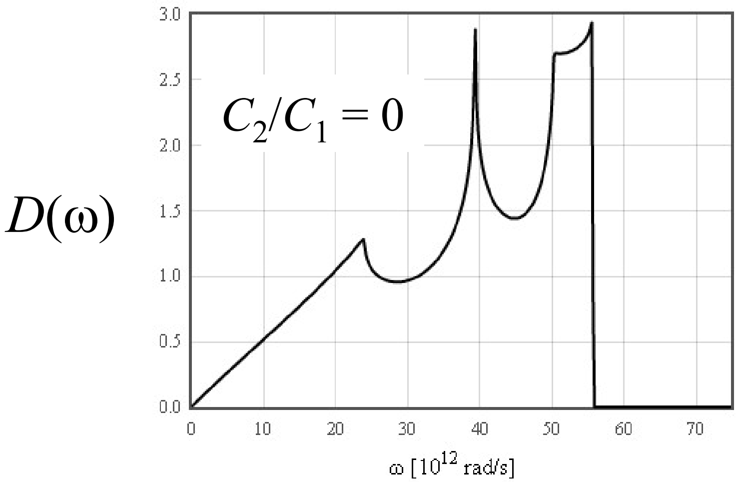
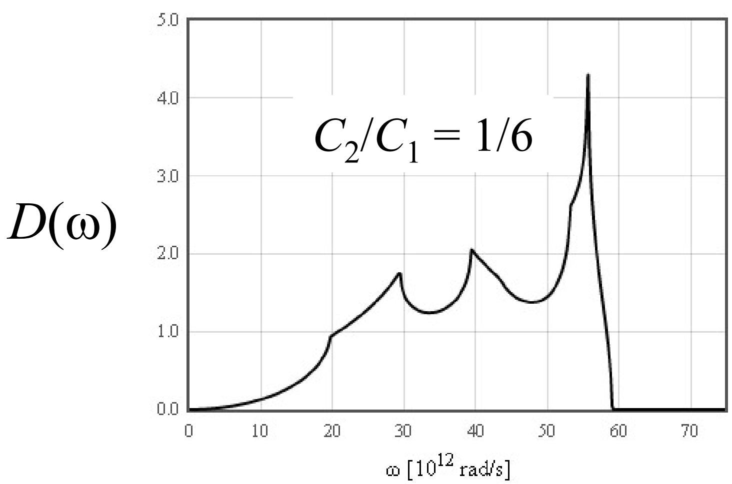
# Phonon DOS Fe



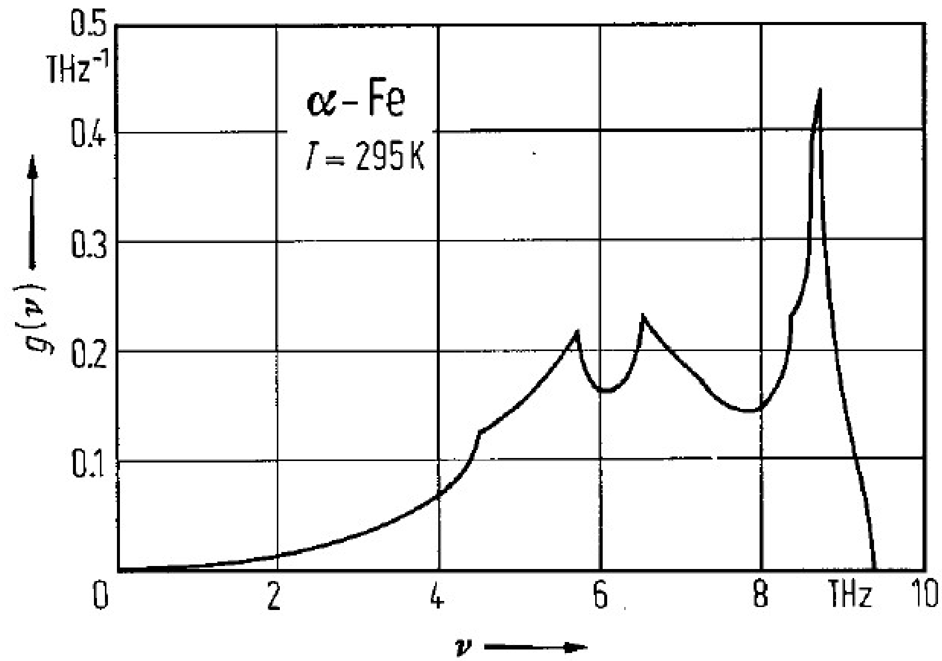




Fig. 3. Fe. Frequency spectrum of α-iron at 295 K calculated from the Born-von Karman force constants of Table 3 Fe [67Mi1].

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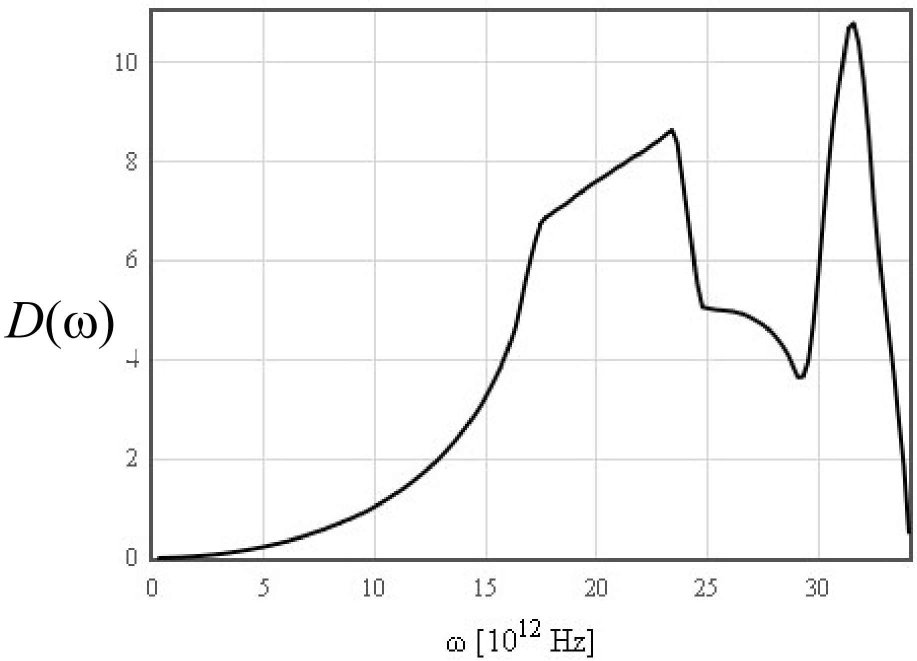
# Phonon DOS fcc



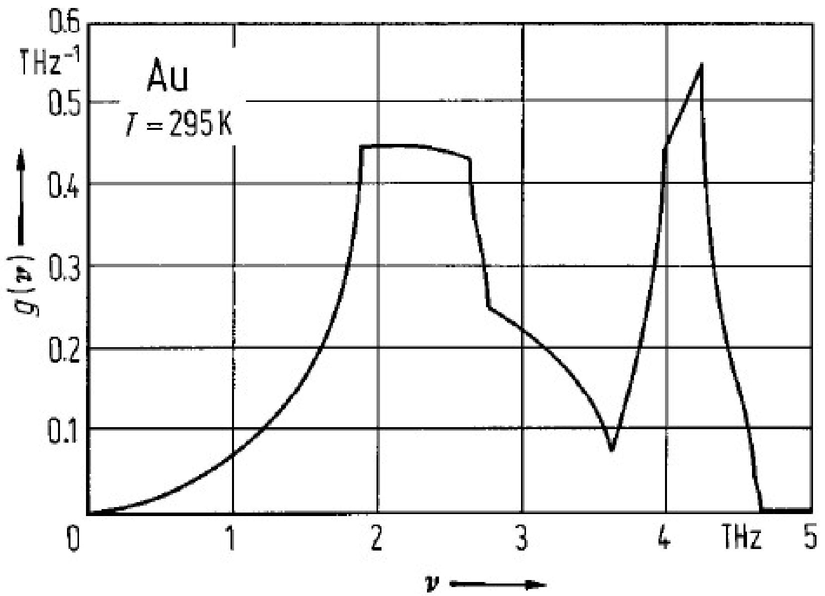
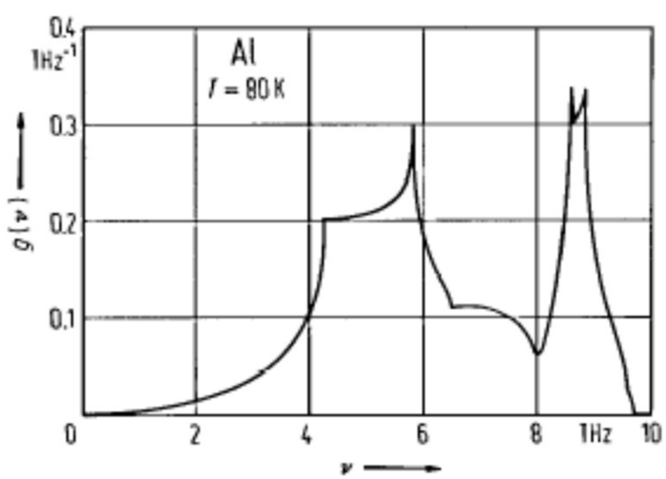
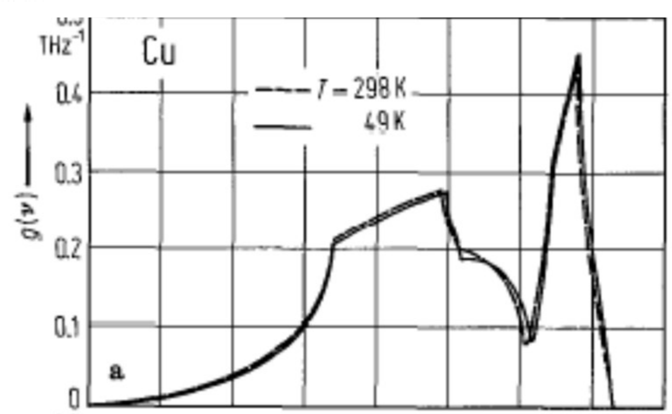




Fig. 2. Au. Frequency distribution calculated from the fourth neighbour general force constant model (M1) of Table 3 Au.

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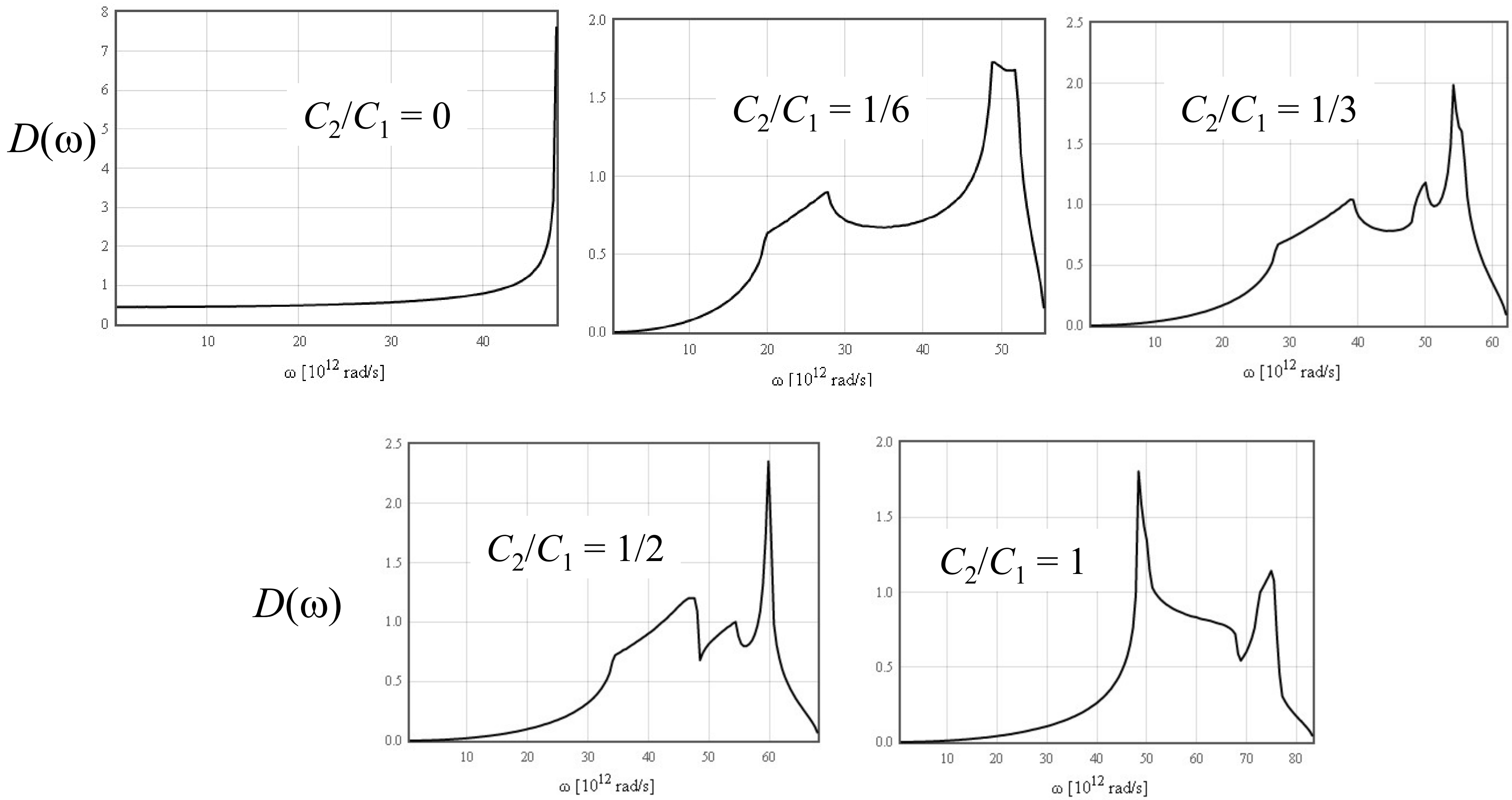
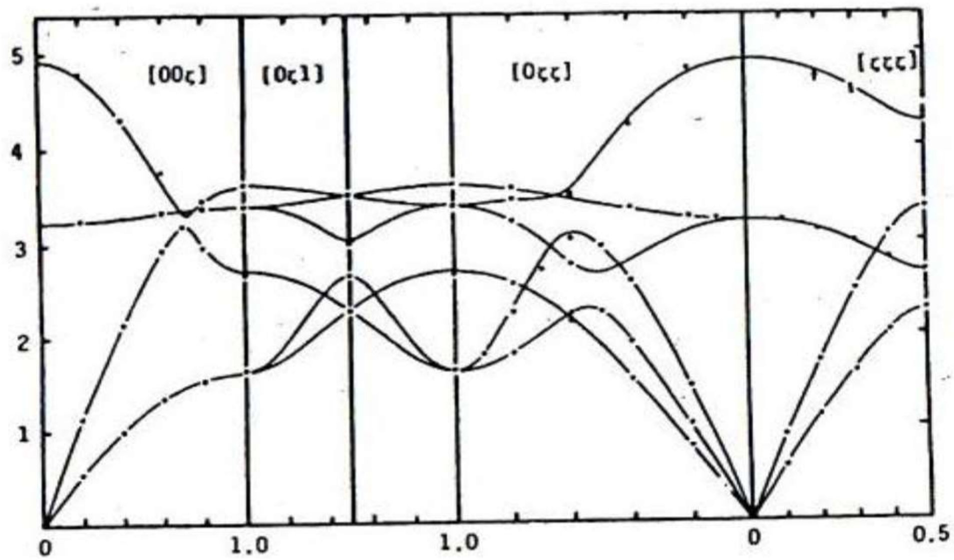
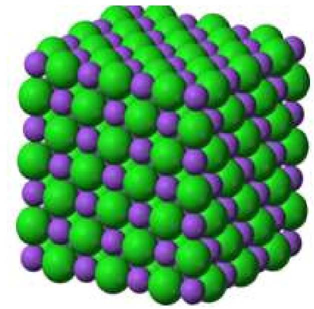
# Next nearest neighbors (simple cubic)



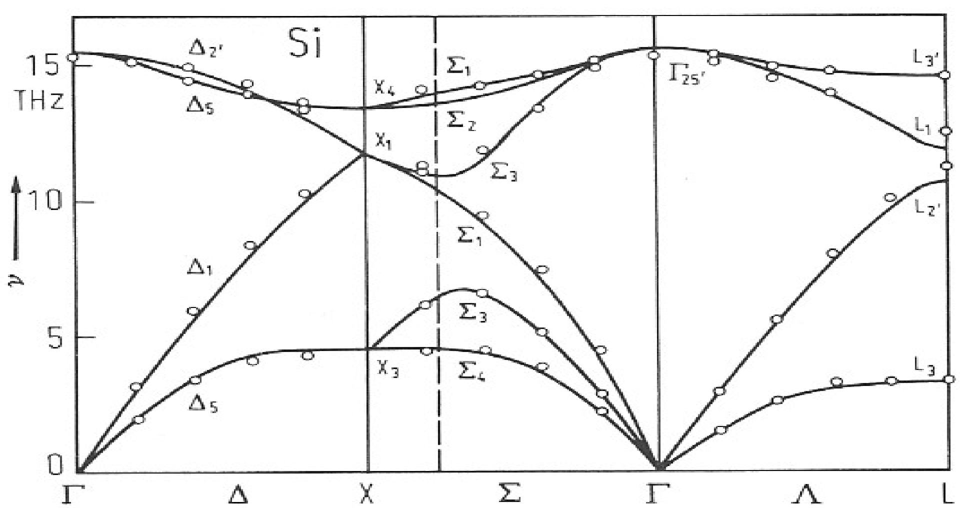

Sometimes the 5th neighbors are included.

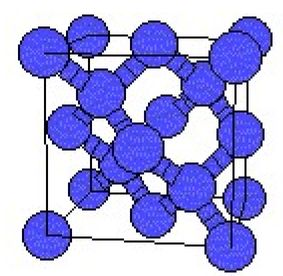
# Two atoms per primitive unit cell



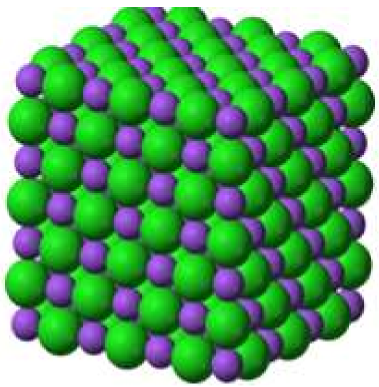
NaCl



Si

# 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:

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

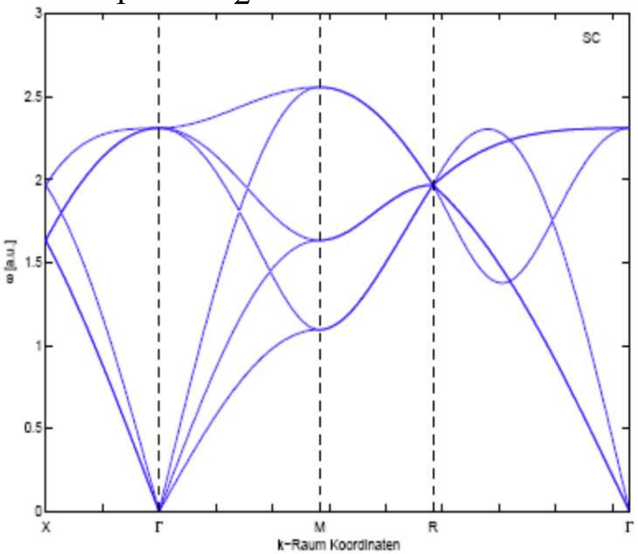
$$M_2 \frac{d^2 v^z_{nml}}{dt^2} = C\left(-2v^z_{nml} + u^z_{n(m+1)(l+1)} + u^z_{(n+1)ml}\right)$$

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

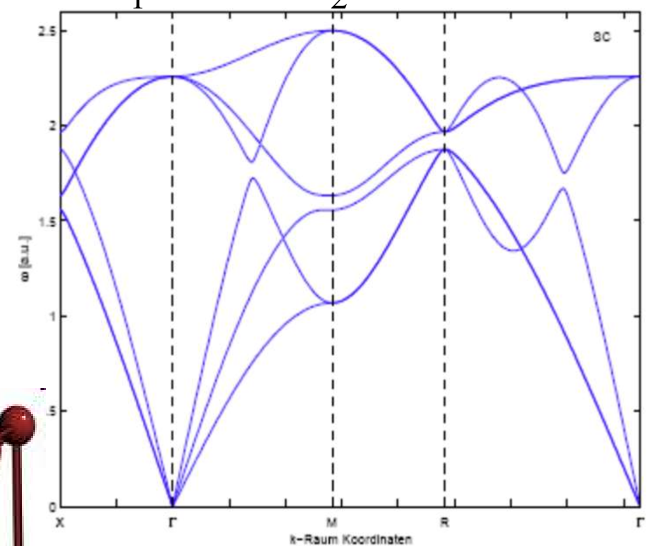
# CsCl

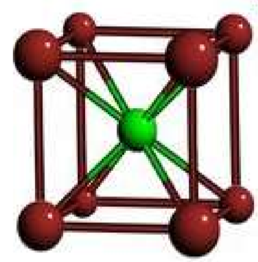
Hannes Brandner

$M_1 = M_2$

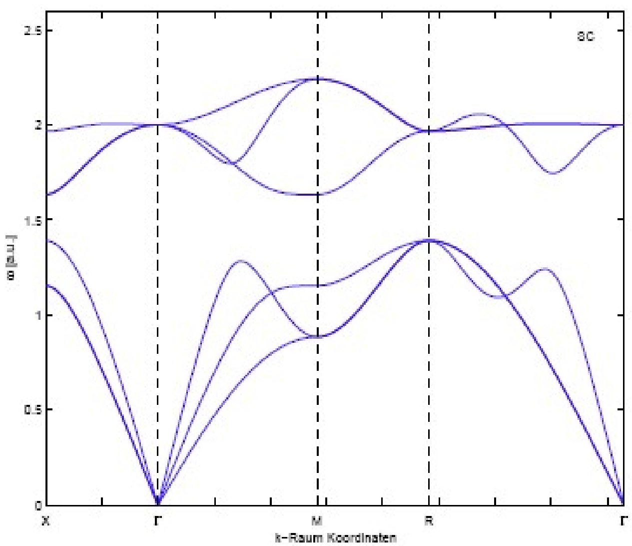


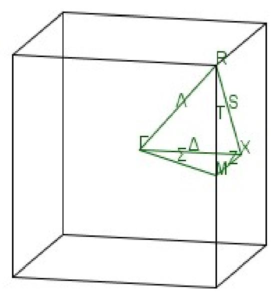

$M_1 = 1.1\, M_2$



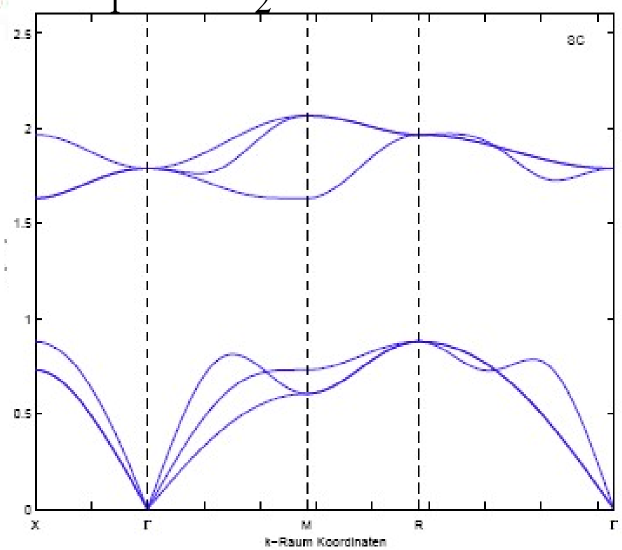



$M_1 = 2M_2$




$M_1 = 5M_2$



# 3 dimensions

*N* atoms

3*N* normal modes

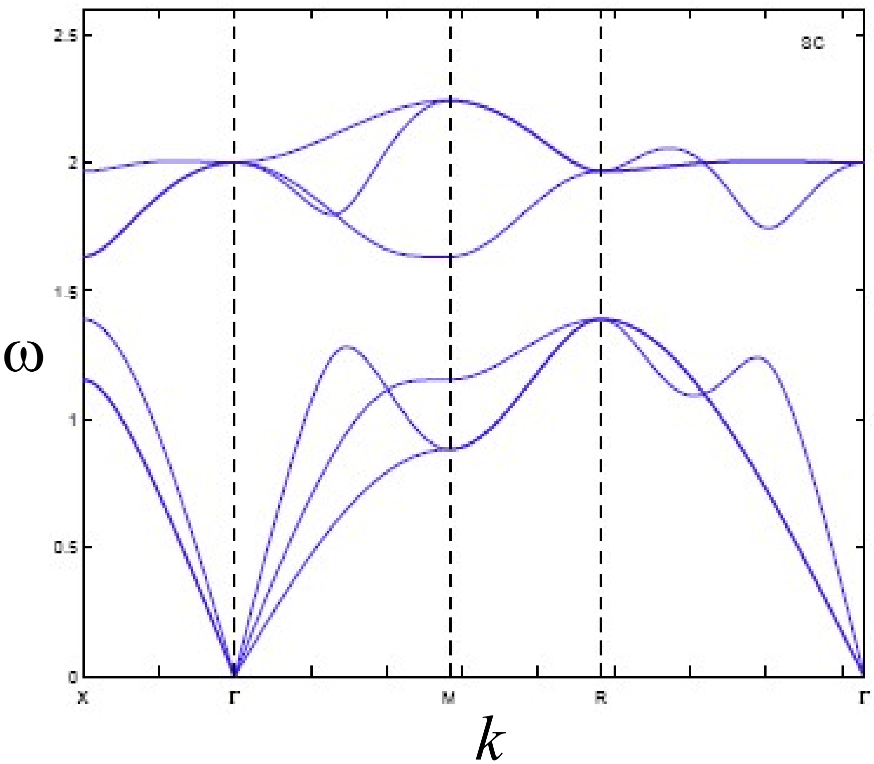
*p* atoms per unit cell

*N*/*p* unit cells = *k* vectors

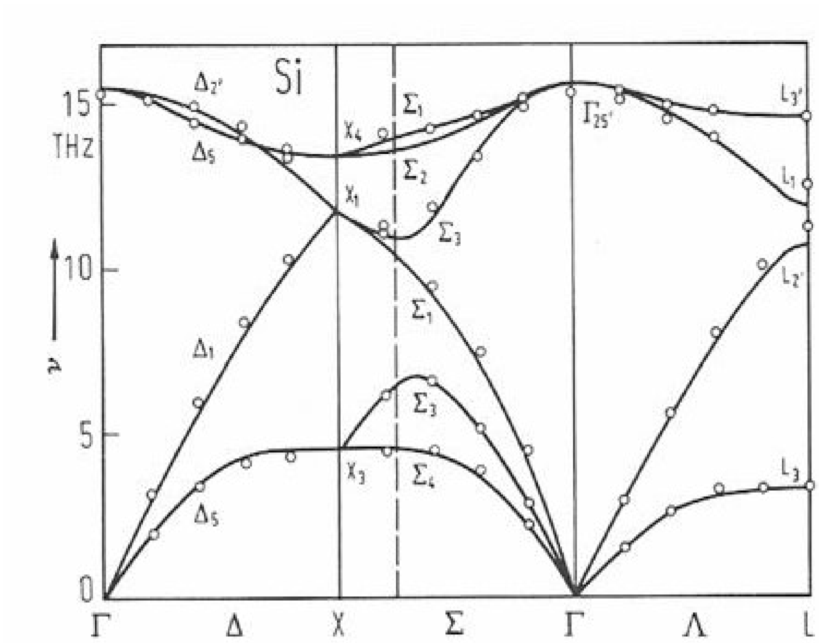
3*p* branches to the dispersion relation

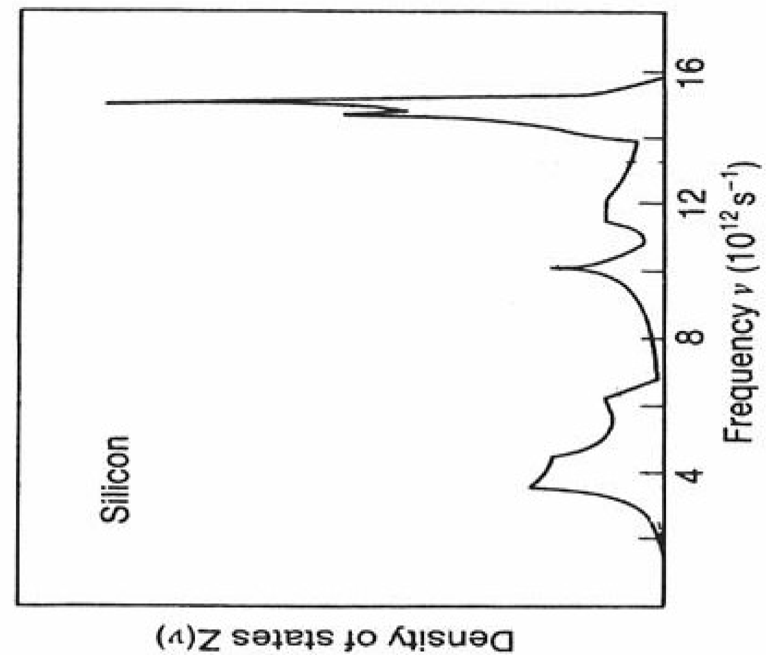
3 acoustic modes (1 longitudinal, 2 transverse)

3*p* - 3 optical modes

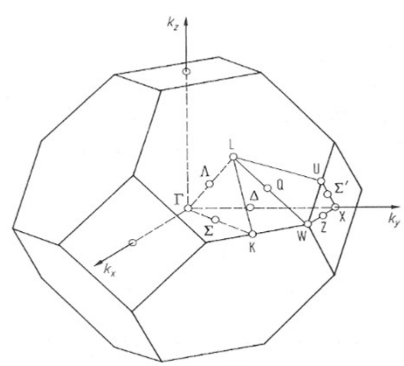


# Silicon phonon dispersion, DOS

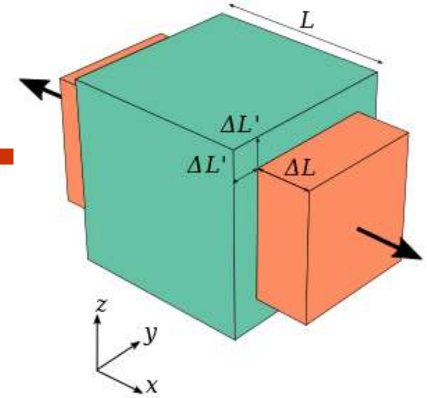



Different speeds of sound for different directions and polarizations causes dispersion of pulses.



# Poisson's ratio

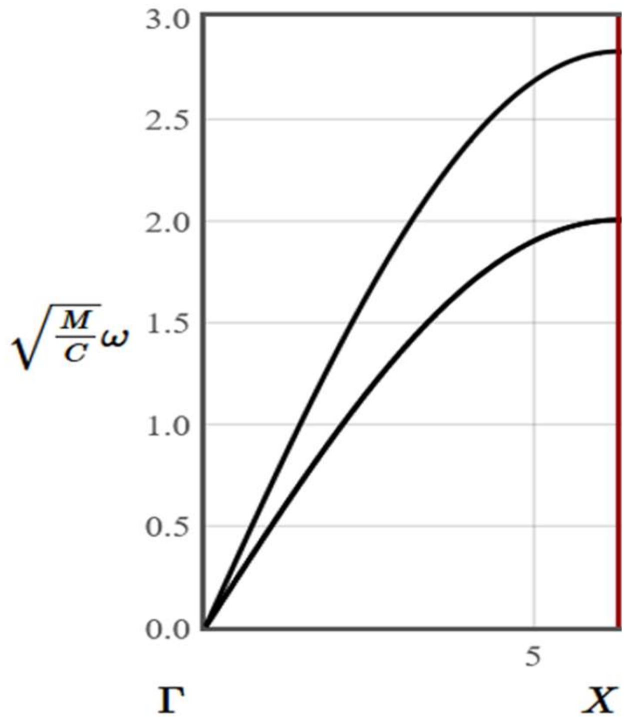



Wikipedia

$E$ - Elastic constant
$\nu$ - Poisson's ratio
$\rho$ - density

$$c_T = \sqrt{\frac{E(1-\nu)}{\rho(1-\upsilon-2\upsilon^2)}}$$

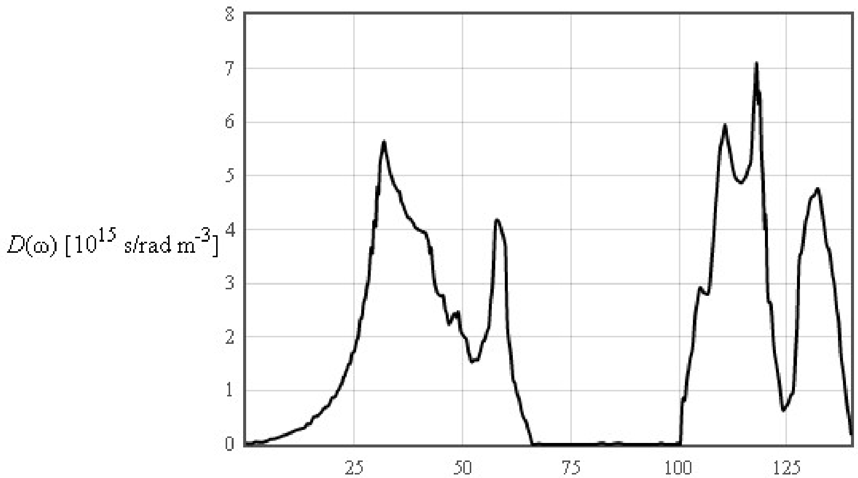
$$c_L = \sqrt{\frac{E}{2\rho(1+\upsilon)}}$$



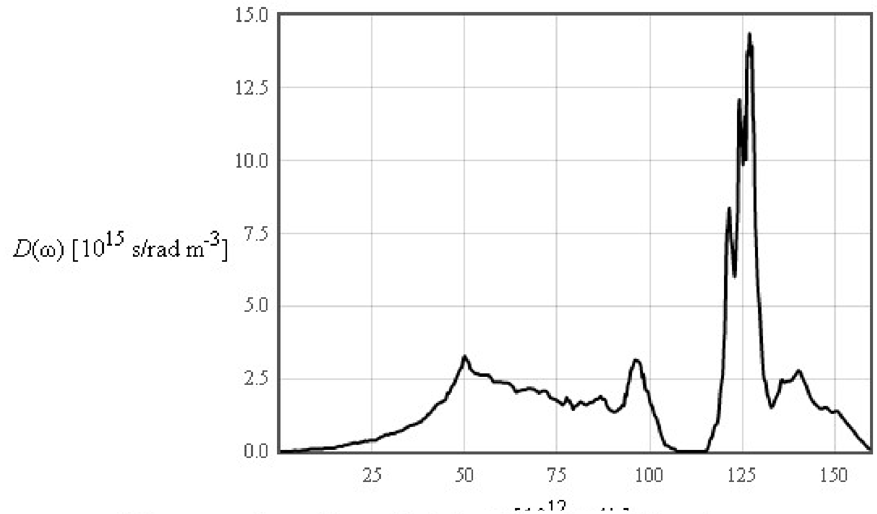

If the density is known, you can determine $E$ and $\nu$.

# Two atoms per primitive unit cell

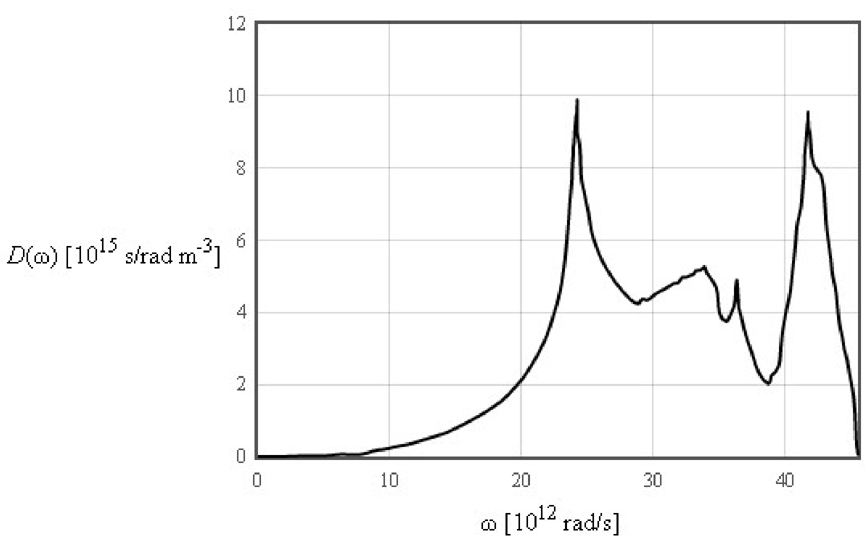
**Phonon density of states for GaN**



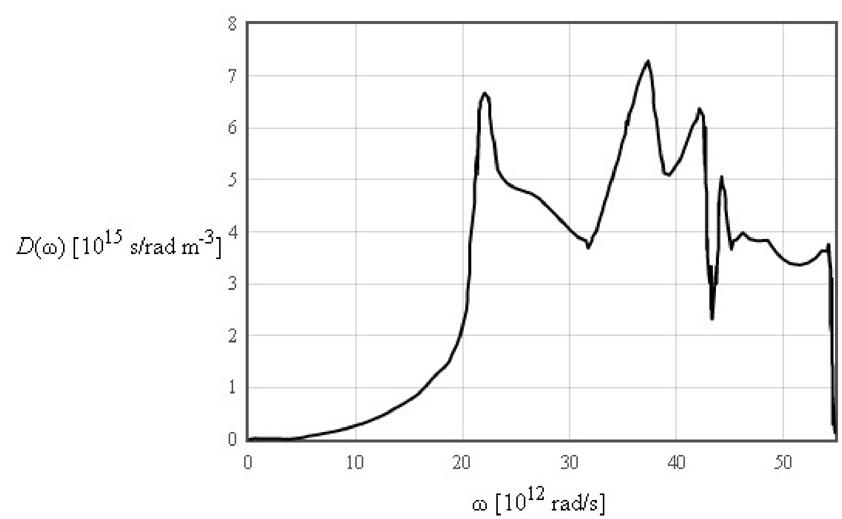

**Phonon density of states for AlN**

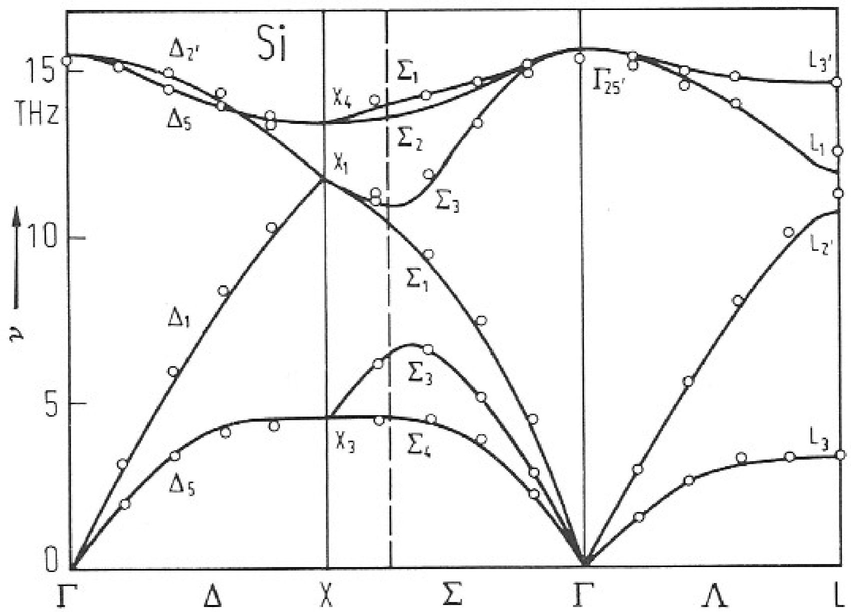


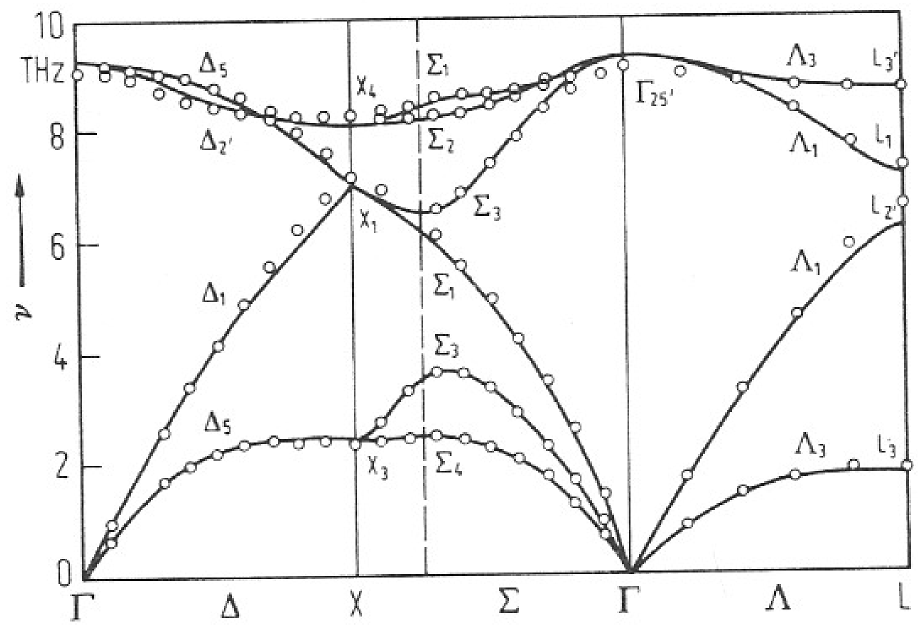

**Phonon density of states for hcp magnesium**



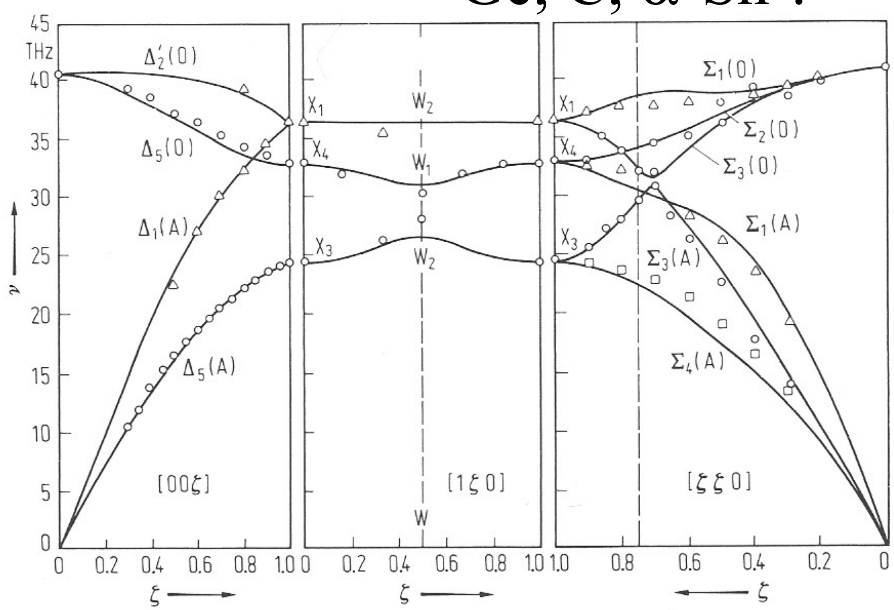

**Phonon density of states for hcp titanium**

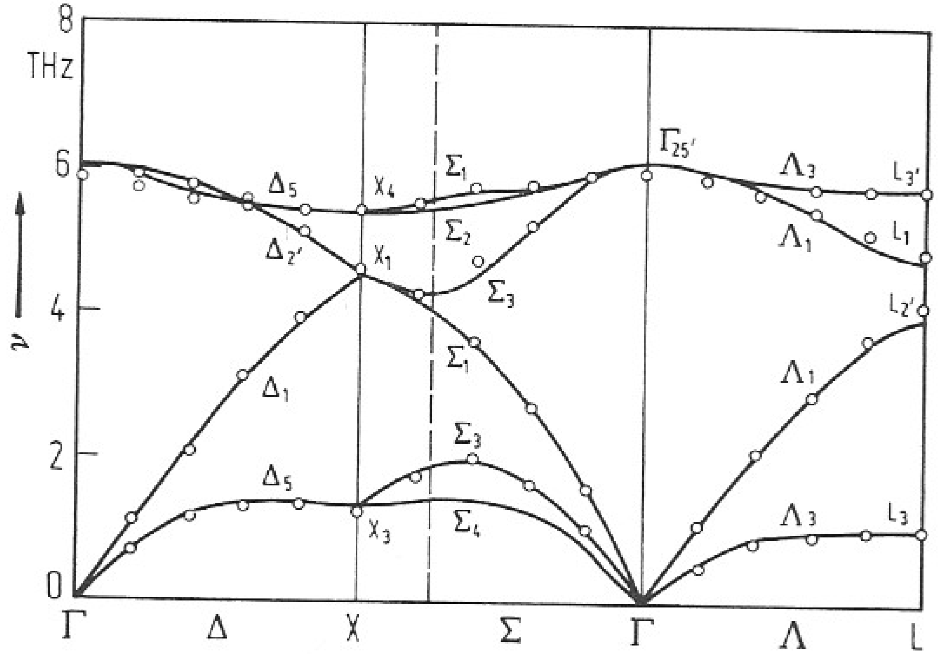



Si
15
THz
10
5
0
ν
Δ2'
Δ5
Δ1
Δ5
X4
X1
X3
Σ1
Σ2
Σ3
Σ1
Σ3
Σ4
Γ25'
L3'
L1
L2'
L3
Γ
Δ
X
Σ
Γ
Λ
L


10
THz
8
6
4
2
0
ν
Δ5
Δ2'
Δ1
Δ5
X4
X1
X3
Σ1
Σ2
Σ3
Σ1
Σ3
Σ4
Γ25'
Λ3
L3'
Λ1
L1
L2'
Λ1
Λ3
L3
Γ
Δ
X
Σ
Γ
Λ
L

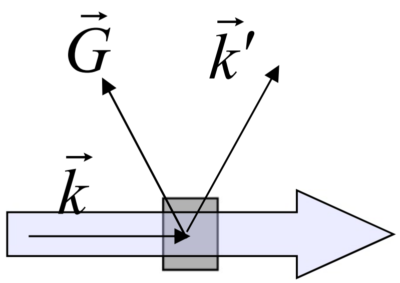
Ge, C, α-Sn ?


45
THz
40
35
30
25
20
15
10
5
0
ν
Δ'2(0)
Δ5(0)
Δ1(A)
Δ5(A)
X1
X4
X3
W2
W1
W2
W
Σ1(0)
Σ2(0)
Σ3(0)
Σ1(A)
Σ3(A)
Σ4(A)
[00ζ]
[1ζ0]
[ζζ0]
0 0.2 0.4 0.6 0.8 1.0
0 0.2 0.4 0.6 0.8 1.0
1.0 0.8 0.6 0.4 0.2 0
ζ
ζ
ζ


8
THz
6
4
2
0
ν
Δ5
Δ2'
Δ1
Δ5
X4
X1
X3
Σ1
Σ2
Σ3
Σ1
Σ3
Σ4
Γ25'
Λ3
L3'
Λ1
L1
L2'
Λ1
Λ3
L3
Γ
Δ
X
Σ
Γ
Λ
L

# Inelastic neutron scattering

Diffraction condition for elastic scattering




$$\vec{k}' = \vec{k} + \vec{G}$$

The whole crystal recoils with momentum $\hbar\vec{G}$

Diffraction condition for inelastic scattering

$$\vec{k}' \pm \vec{K}_{ph} = \vec{k} + \vec{G} \qquad \frac{\hbar^2 k'^2}{2m_n} \pm \hbar\omega_{ph} = \frac{\hbar^2 k^2}{2m_n} + \cancelto{0}{\frac{\hbar^2 G^2}{2m_{crystal}}}$$

$\vec{K}_{ph}$ is the phonon momentum

Phonon dispersion relations are determined experimentally by inelastic neutron diffraction

# long wavelength limit

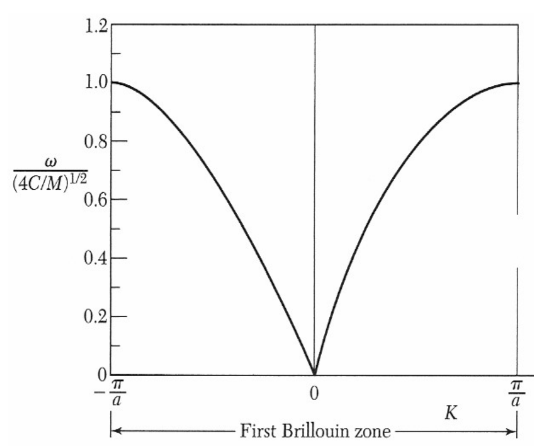
discrete version of wave equation

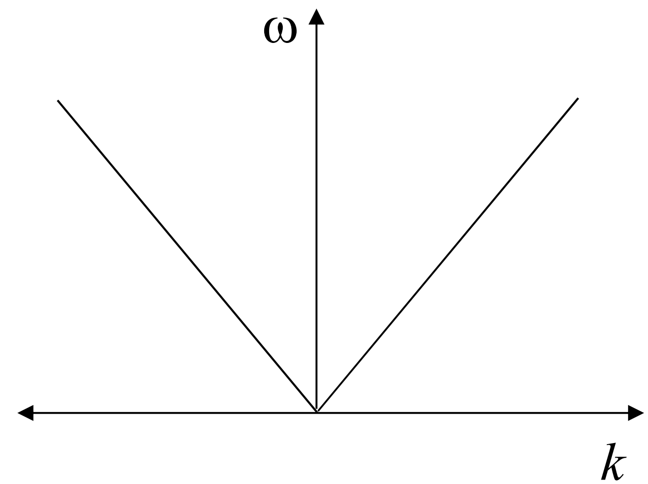
$$m\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$$

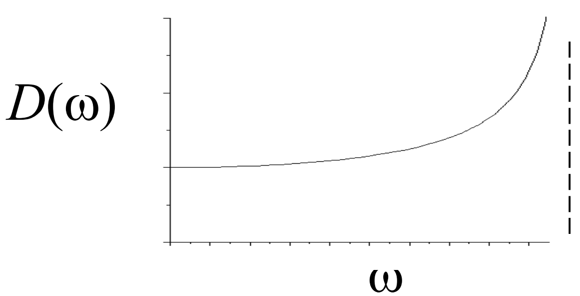
1-d wave equation

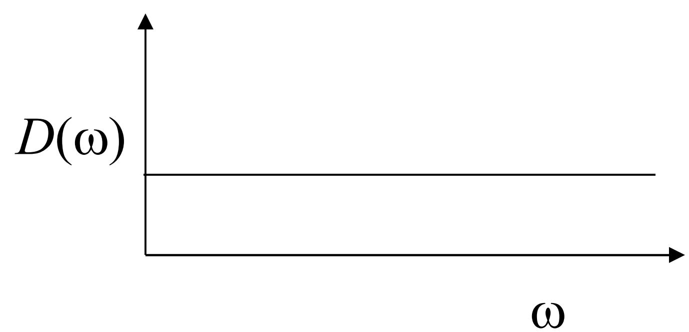
$$\frac{d^2u}{dt^2} = c^2\frac{d^2u}{dx^2}$$

The solutions to the linear chain are the same as the solutions to the wave equation for $|k| << \pi/a$.



# Phonons - long wavelength, low temperature limit

At low $T$, there are only long wave length states occupied.

3 polarizations

Density of states: $$D(\omega)d\omega = \frac{3\omega^2}{2c^3\pi^2}d\omega.$$

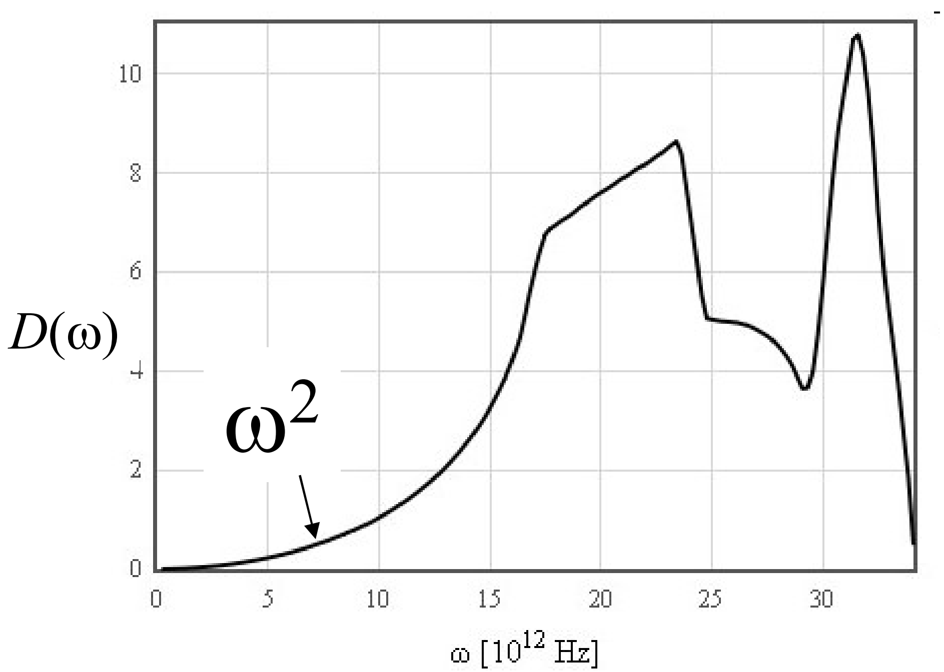
Specific heat of insulators at low temperatures

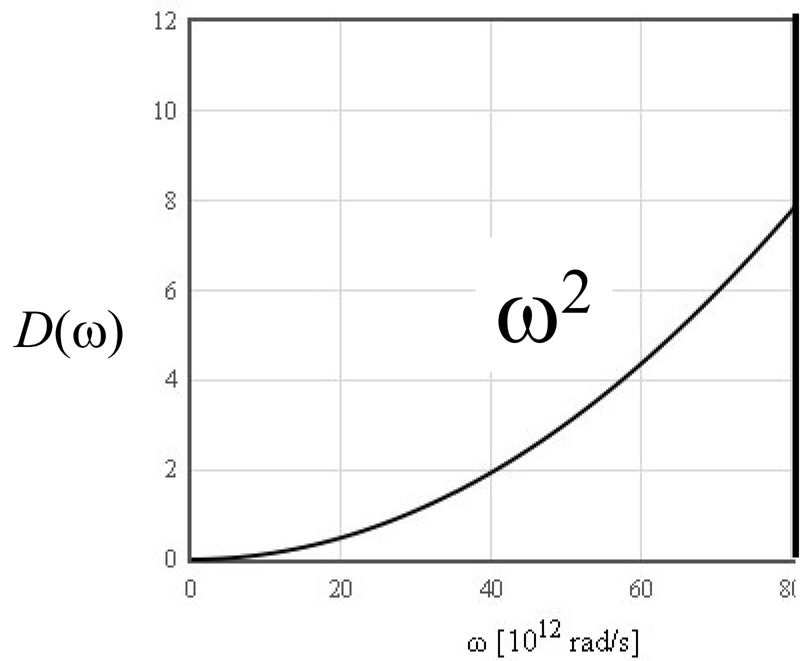
$$c_v = \frac{16\pi^5 k_B^4 T^3}{5c^3h^3} \quad \text{J K}^{-1}\ \text{m}^{-1}$$

Speed of sound

| | |
|---|---|
| $I = \frac{2\pi^5 k_B^4 T^4}{15c^2h^3} = \sigma T^4$ | [J m$^{-2}$ s$^{-2}$] |
| $u(\lambda) = \frac{8\pi hc}{\lambda^5\left(\exp\left(\frac{hc}{\lambda k_B T}\right)-1\right)}$ | [J/m$^4$] |
| $u = \frac{4\sigma T^4}{c}$ | [J/m$^3$] |
| $c_v = \frac{16\sigma T^3}{c}$ | [J K$^{-1}$ m$^{-3}$] |
| $f = \frac{-4\sigma T^4}{3c}$ | [J/m$^3$] |
| $s = \frac{16\sigma T^3}{3c}$ | [J K$^{-1}$ m$^{-3}$] |
| $P = \frac{4\sigma T^4}{3c}$ | [N/m$^2$] |

# long wavelength, low temperature limit



# Empty lattice approximation

Use the speed of sound instead of the speed of light.

3 acoustic branches
3$p$ - 3 optical branches