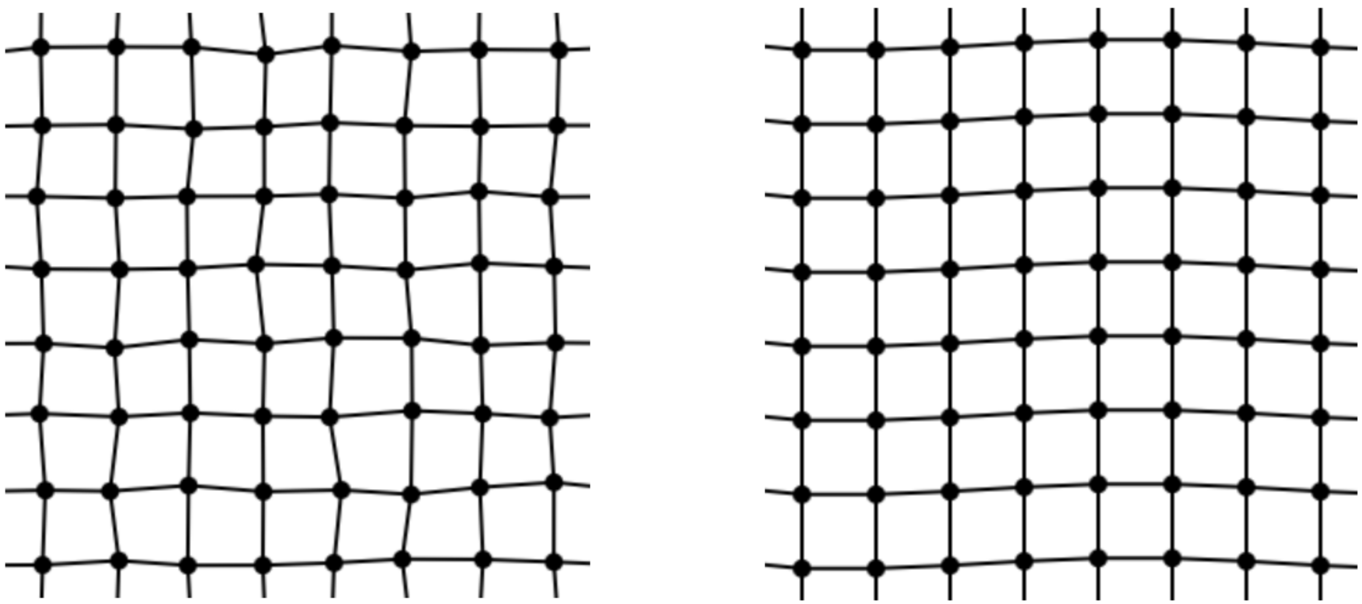
15. Phonons

May 15, 2018

Normal modes



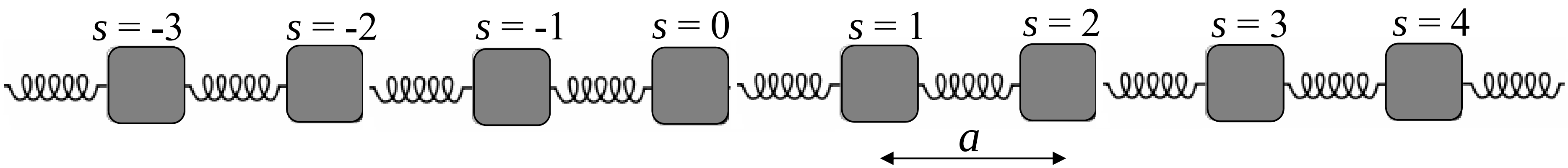
The motion of the atoms can be described in terms of normal modes.

In a normal mode, all atoms oscillate at the same frequency ω.

The energy in a normal mode is quantized, $E = \hbar\omega(n + \frac{1}{2})$.

n is the number of phonons in that normal mode.

Linear Chain



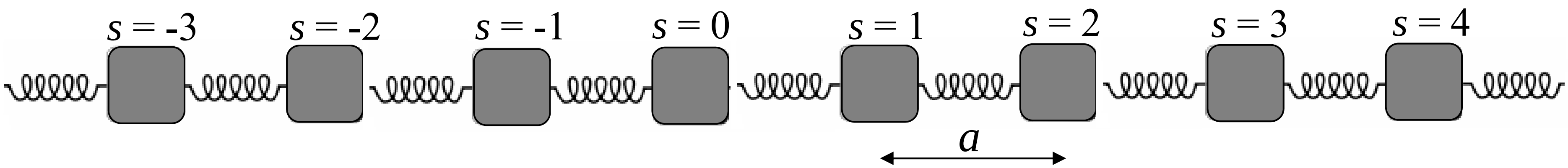
$$m\frac{d^2u_s}{dt^2} = C(u_{s+1}-u_s) - C(u_s - u_{s-1}) = C(u_{s+1} - 2u_s + u_{s-1})$$

Assume every atom oscillates with the same frequency $u_s = A_s e^{-i\omega t}$

$$\begin{bmatrix} 2C-\omega^2 m & -C & 0 & 0 & 0 & -C \\ -C & 2C-\omega^2 m & -C & 0 & 0 & 0 \\ 0 & -C & 2C-\omega^2 m & -C & 0 & 0 \\ 0 & 0 & -C & 2C-\omega^2 m & -C & 0 \\ 0 & 0 & 0 & -C & 2C-\omega^2 m & -C \\ -C & 0 & 0 & 0 & -C & 2C-\omega^2 m \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \\ A_6 \end{bmatrix} = 0$$

$$\left[\left(2C-\omega^2 m\right)\mathrm{I} - C\left(\mathrm{T}+\mathrm{T}^{-1}\right)\right]\vec{A} = 0.$$

Normal modes are eigen functions of T



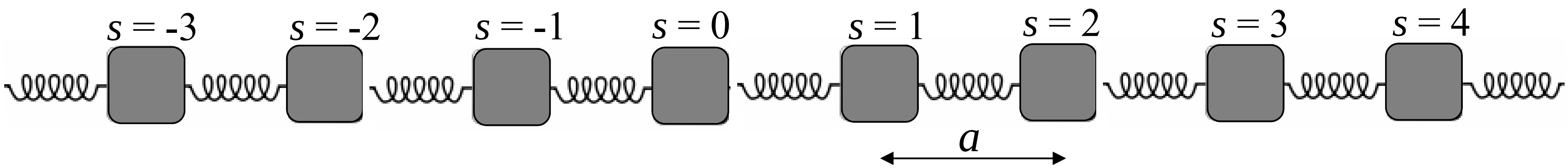
solutions are eigenfunctions of the translation operator

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

$$Tu_s = A_k e^{i(k(s+1)a - \omega t)} = e^{ika} A_k e^{i(ksa - \omega t)} = e^{ika} u_s$$

N atoms, *N* normal modes, *N* eigenvectors of the translation operator, *N* allowed values of *k* in the first Brillouin zone.

Linear Chain



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

solutions: $$u_s = A_k e^{i(ksa-\omega t)}$$

$$-\omega^2 m e^{i(ksa-\omega t)} = C(e^{i(k(s+1)a-\omega t)} - 2e^{i(ksa-\omega t)} + e^{i(k(s-1)a-\omega t)})$$

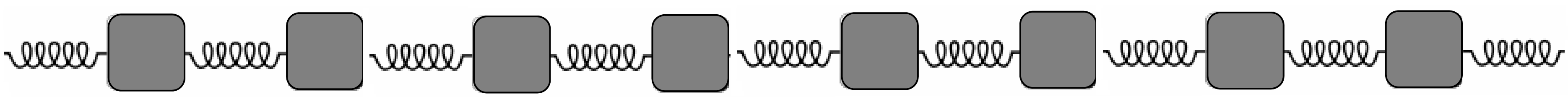
$$-\omega^2 m = C(e^{ika} - 2 + e^{-ika})$$

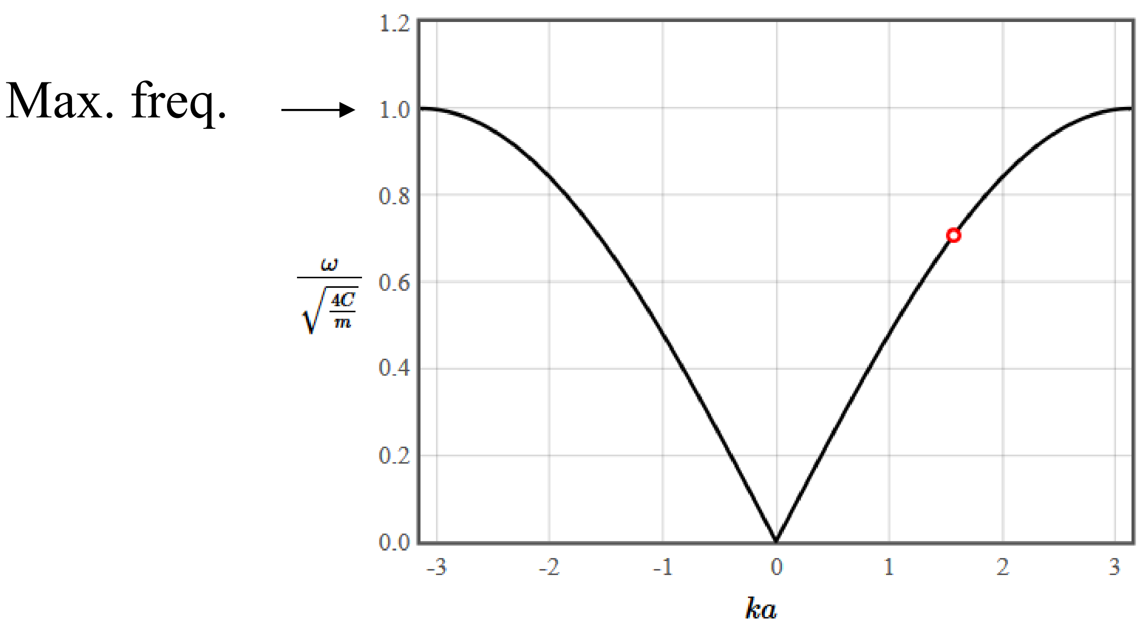
$$\omega^2 m = 2C(1-\cos(ka))$$

$$\sin^2\frac{ka}{2} = \frac{1}{2}(1-\cos ka)$$

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

Linear Chain - dispersion relation

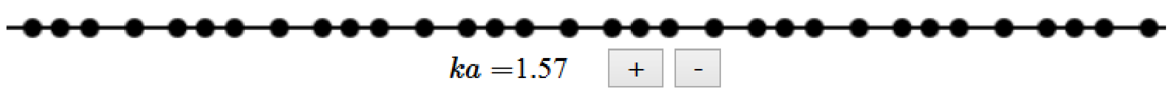




$$m\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$$

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

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

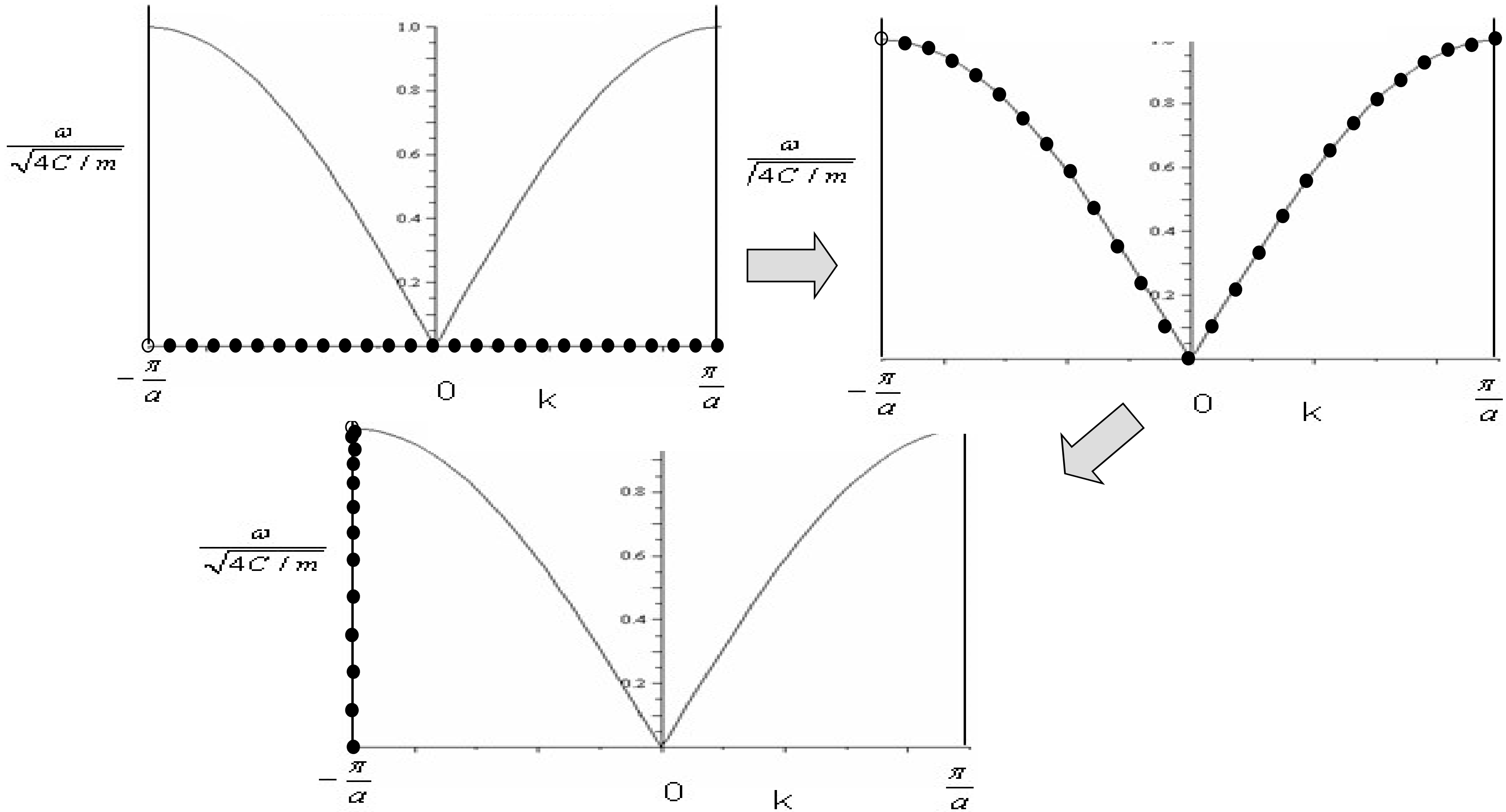


$$\text{speed of sound} = \sqrt{\frac{C}{m}}a$$

Linear Chain - density of states

Determine the density of states numerically

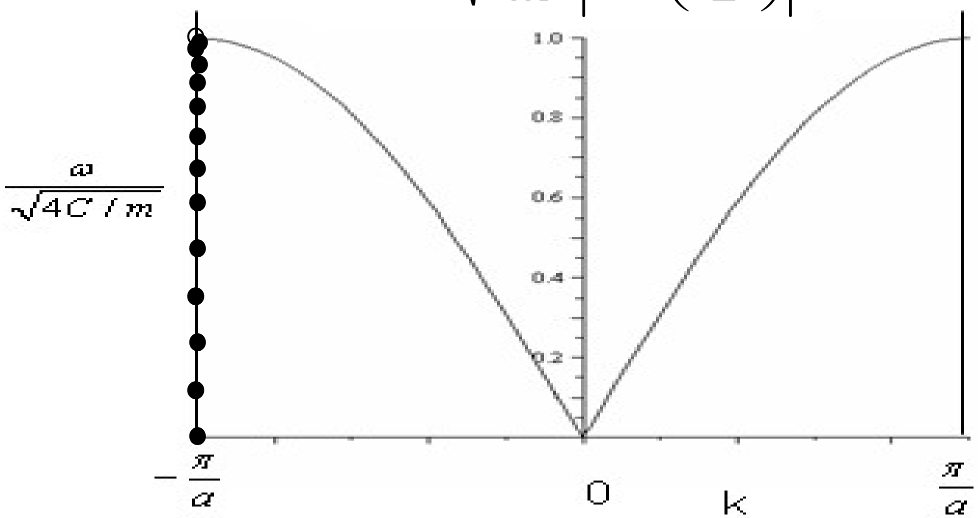
$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



Linear Chain - density of states

This case is an exception where the density of states can be determined analytically.

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



for every k calculate the frequency

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

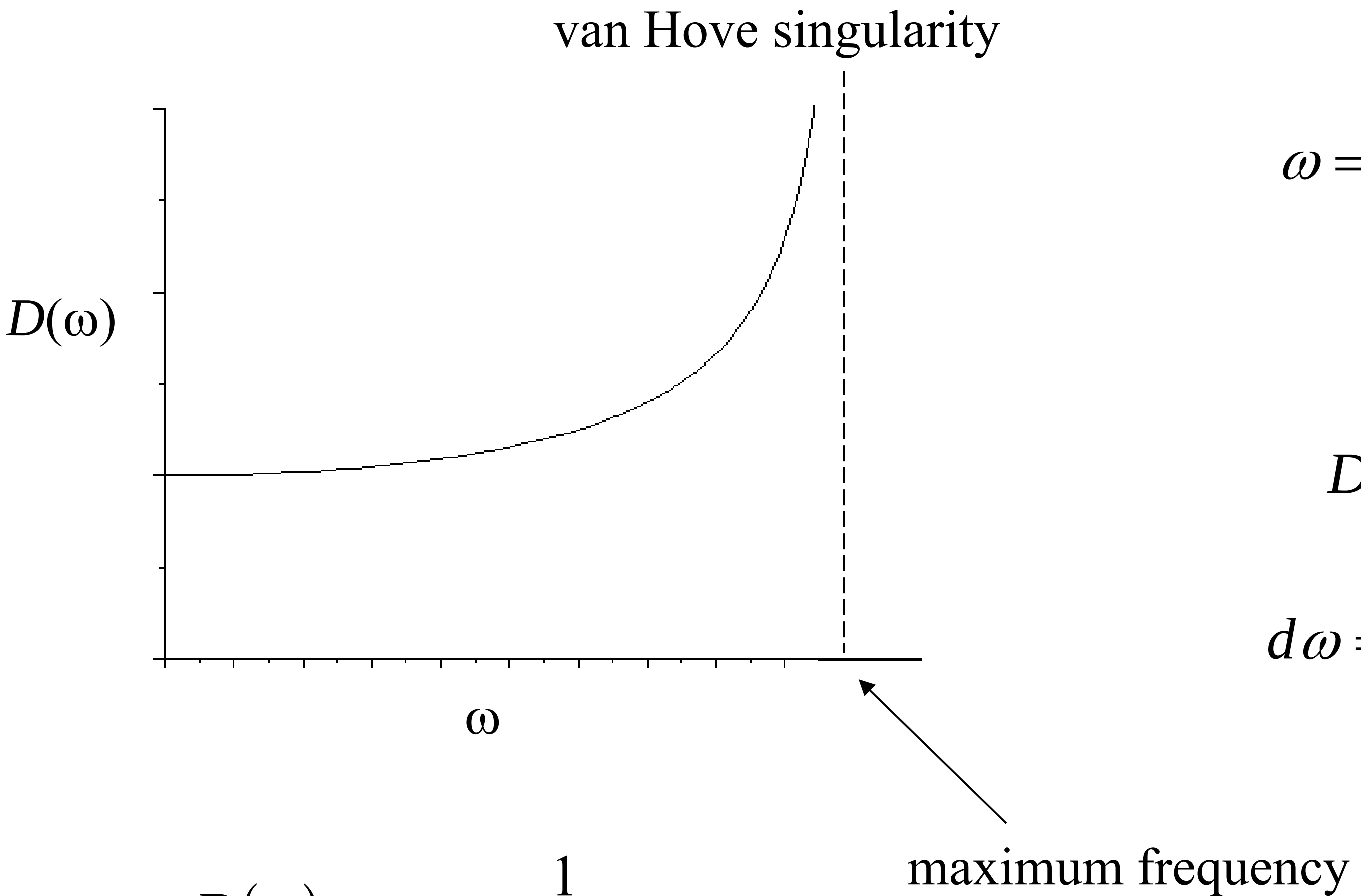
$$D(k) = \frac{1}{\pi}$$

$$D(\omega) = D(k)\frac{dk}{d\omega}$$

$$d\omega = a\sqrt{\frac{C}{m}}\cos\left(\frac{ka}{2}\right)dk$$

$$D(\omega) = \frac{1}{\pi a\sqrt{\frac{C}{m}}\sqrt{1-\frac{\omega^2 m}{4C}}}$$

density of states



$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

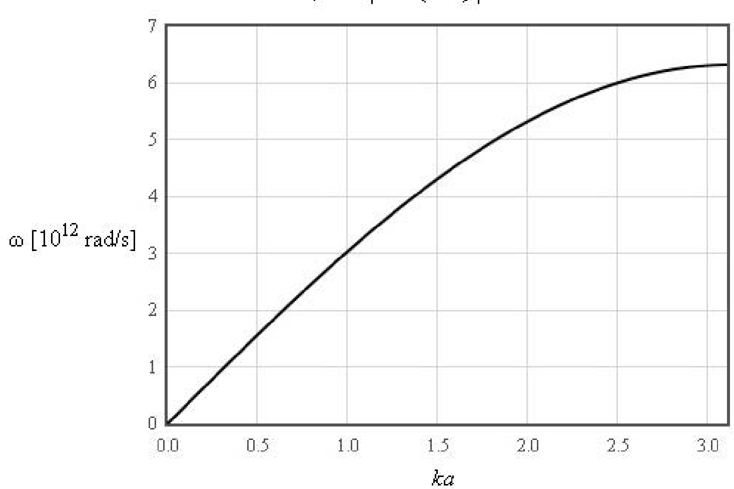
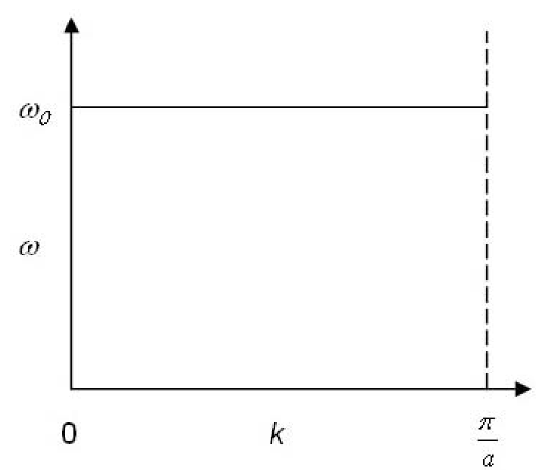
$$D(k) = \frac{1}{\pi}$$

$$D(k)dk = D(\omega)d\omega$$

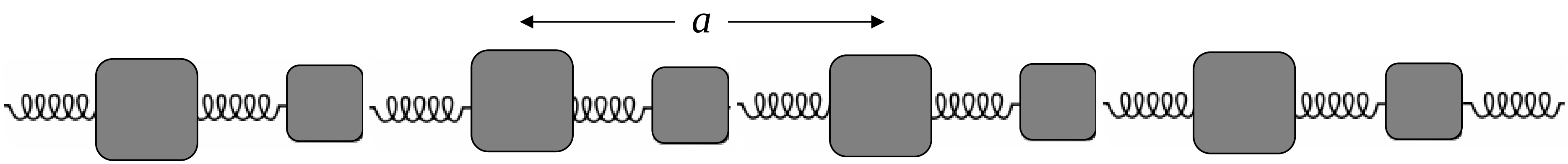
$$d\omega = a\sqrt{\frac{C}{m}}\cos\left(\frac{ka}{2}\right)dk$$

$$D(\omega) = \frac{1}{\pi a\sqrt{\frac{C}{m}}\sqrt{1-\frac{\omega^2 m}{4C}}}$$

Phonons

	Linear Chain $$m\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$$	**Einstein Model** Einstein assumed that all of the $3N$ normal modes of a crystal containing N atoms have the same frequency ω_0. This is not a good model for the dispersion relation but it does a reasonable job in describing the specific heat.	Debye used the l… ω^2 up to a cut-off… go to zero. The c…
Eigenfunction solutions	$u_s = A_k e^{i(ksa-\omega t)}$		
Dispersion relation	$$\omega = \sqrt{\frac{4C}{m}}\left\|\sin\left(\frac{ka}{2}\right)\right\|$$ 		

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

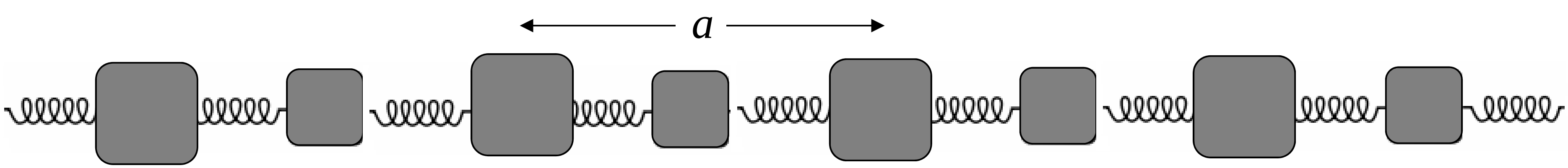
$$u_s = u_k e^{i(ksa - \omega t)}$$

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

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

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

Linear chain M_1 and M_2



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

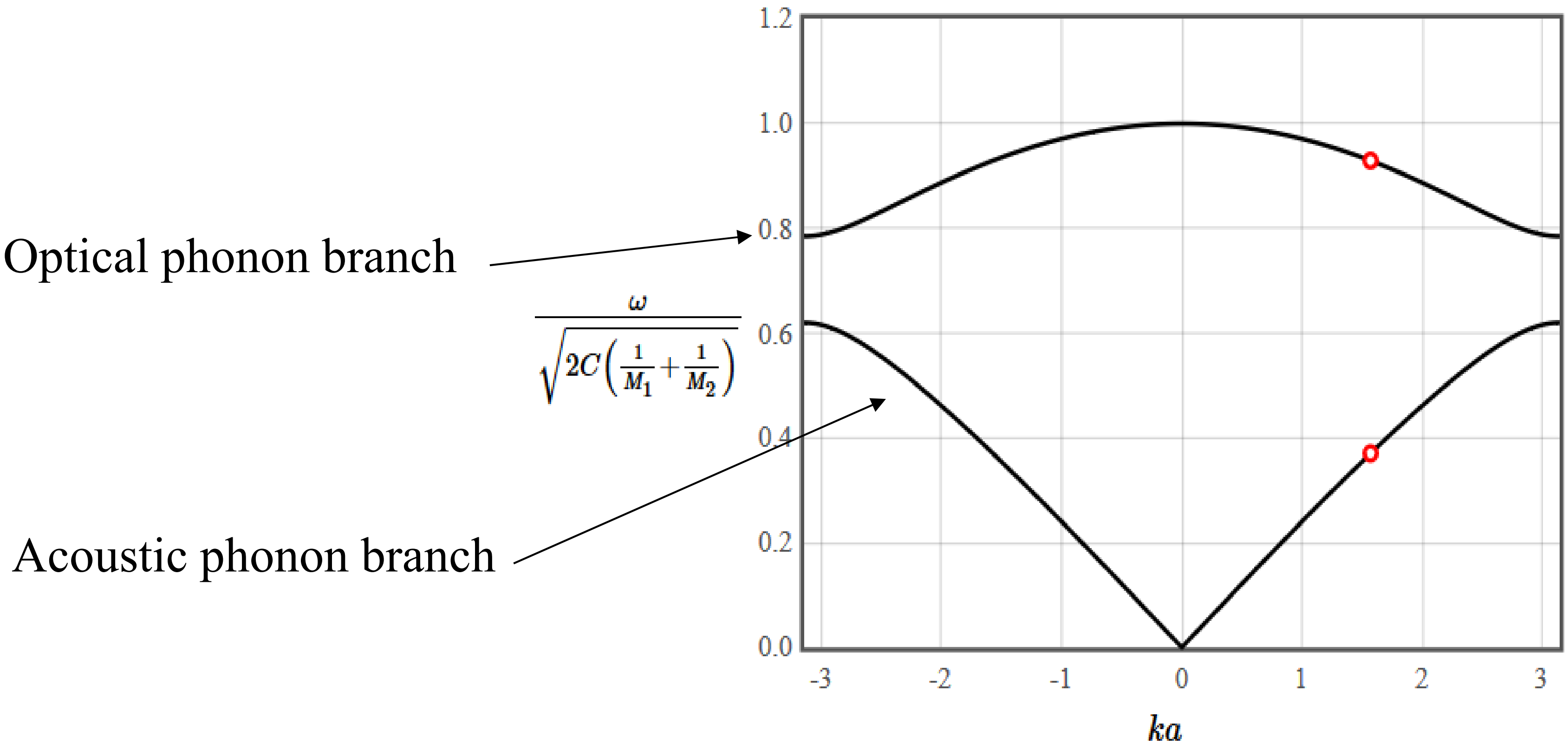
$$-\omega^2 M_2 v_k = C u_k (1+\exp(ika)) - 2C v_k$$

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

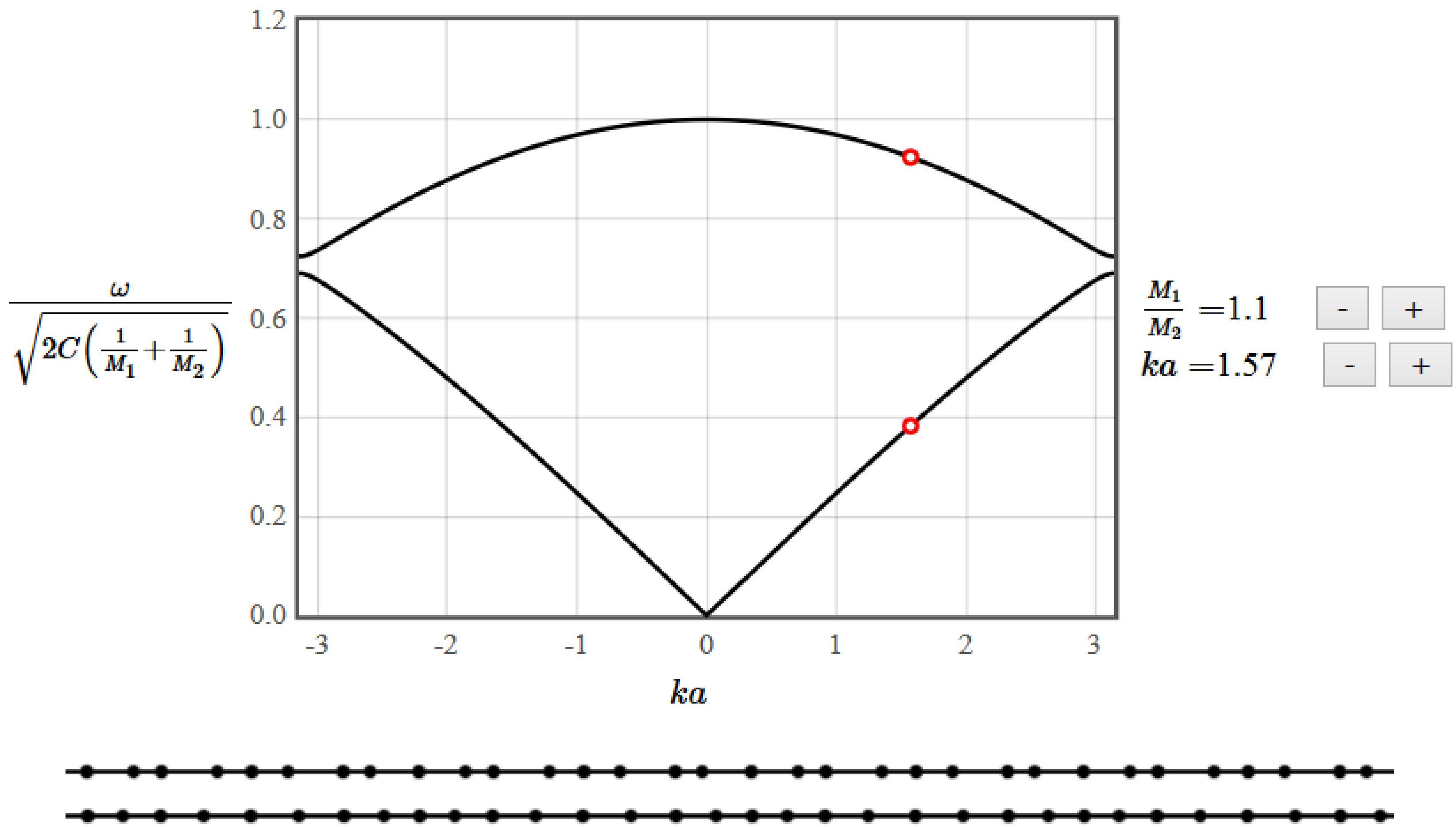
$$M_1 M_2 \omega^4 - 2C\left(M_1 + M_2\right)\omega^2 + 2C^2\left(1-\cos(ka)\right) = 0$$

dispersion relation

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

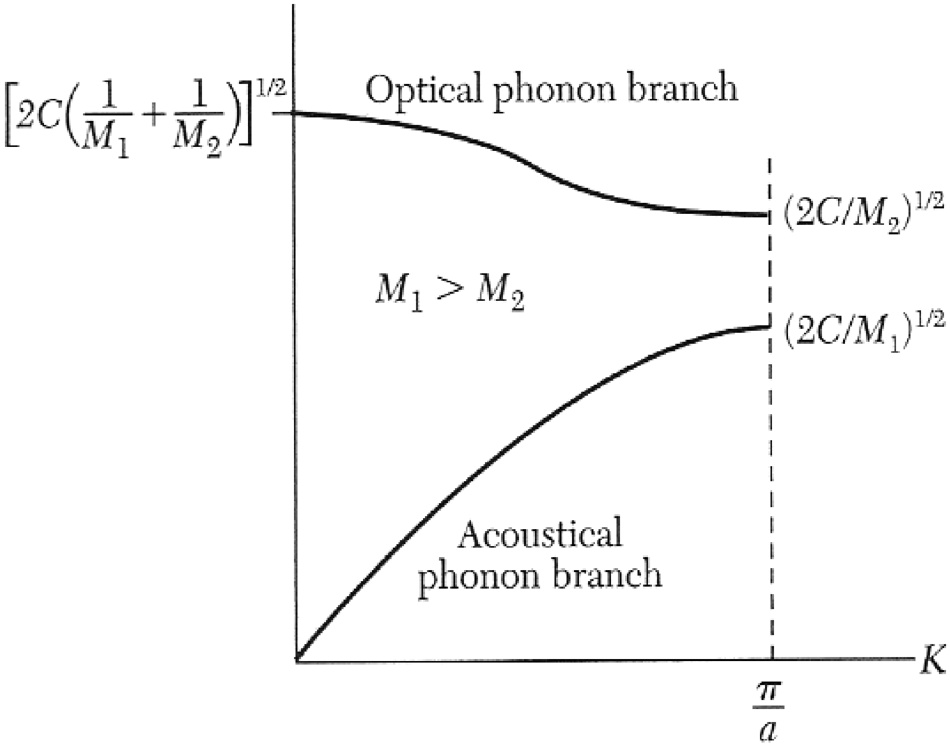


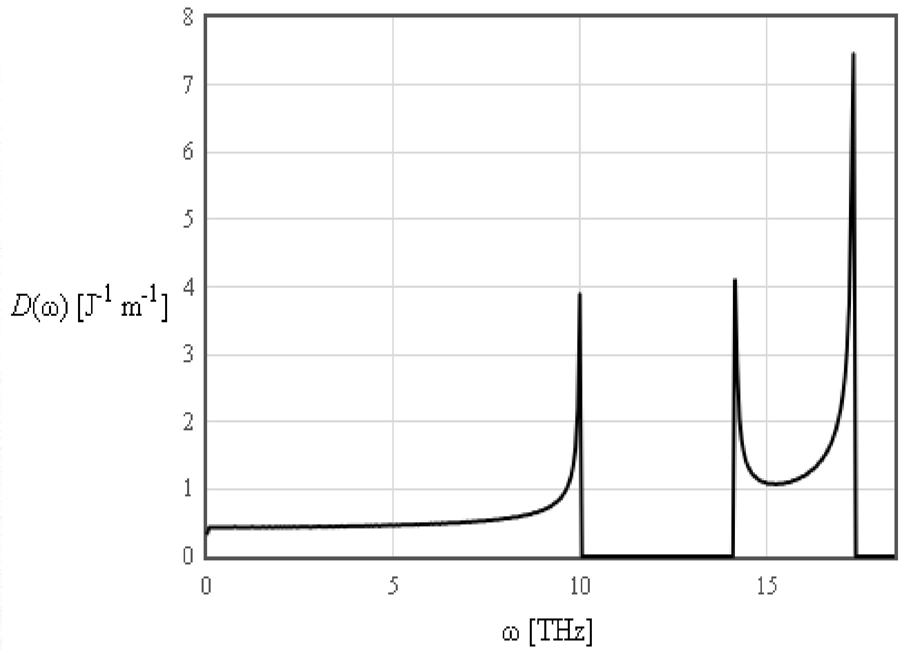
normal modes



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

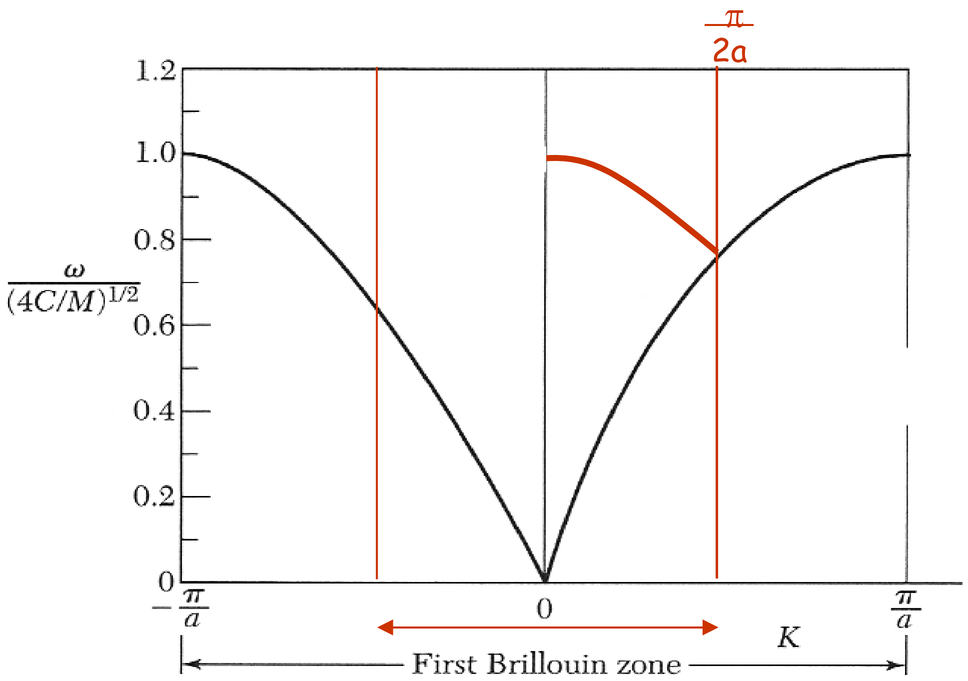
density of states

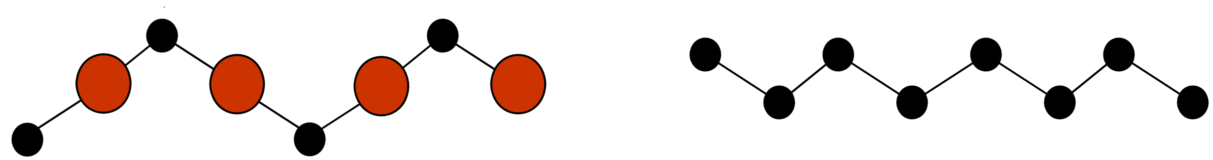




$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2 ka}{M_1 M_2}}$$

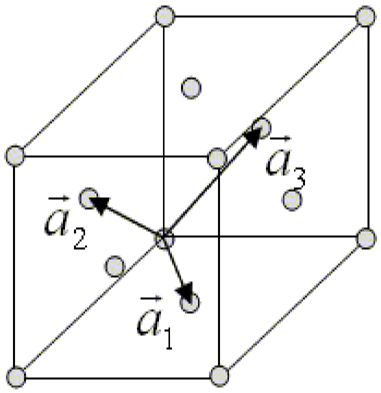
Linear chain M_1 and M_2





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

fcc



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

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

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

$$m\frac{d^2u^x_{lmn}}{dt^2} = \frac{C}{2}\Big[\left(u^x_{l+1mn} - u^x_{lmn}\right) + \left(u^x_{l-1mn} - u^x_{lmn}\right) + \left(u^x_{lm+1n} - u^x_{lmn}\right) + \left(u^x_{lm-1n} - u^x_{lmn}\right)$$

$$+\left(u^x_{l+1mn-1} - u^x_{lmn}\right) + \left(u^x_{l-1mn+1} - u^x_{lmn}\right) + \left(u^x_{lm+1n-1} - u^x_{lmn}\right) + \left(u^x_{lm-1n+1} - u^x_{lmn}\right)$$

$$+\left(u^y_{l+1mn} - u^y_{lmn}\right) + \left(u^y_{l-1mn} - u^y_{lmn}\right) - \left(u^y_{lm+1n-1} - u^y_{lmn}\right) - \left(u^y_{lm-1n+1} - u^y_{lmn}\right)$$

$$+\left(u^z_{lm+1n} - u^z_{lmn}\right) + \left(u^z_{lm-1n} - u^z_{lmn}\right) - \left(u^z_{l+1mn-1} - u^z_{lmn}\right) - \left(u^z_{l-1mn+1} - u^z_{lmn}\right)\Big]$$

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

Normal modes are eigenfunctions of T

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

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

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

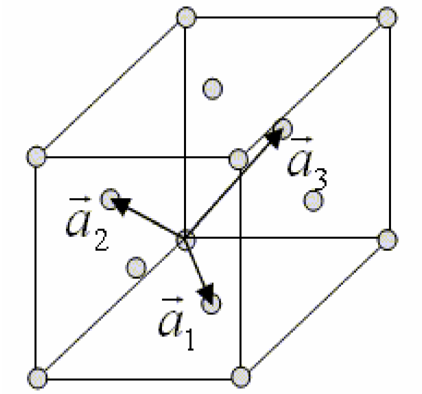
These are eigenfunctions of T.

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

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

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

fcc



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

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

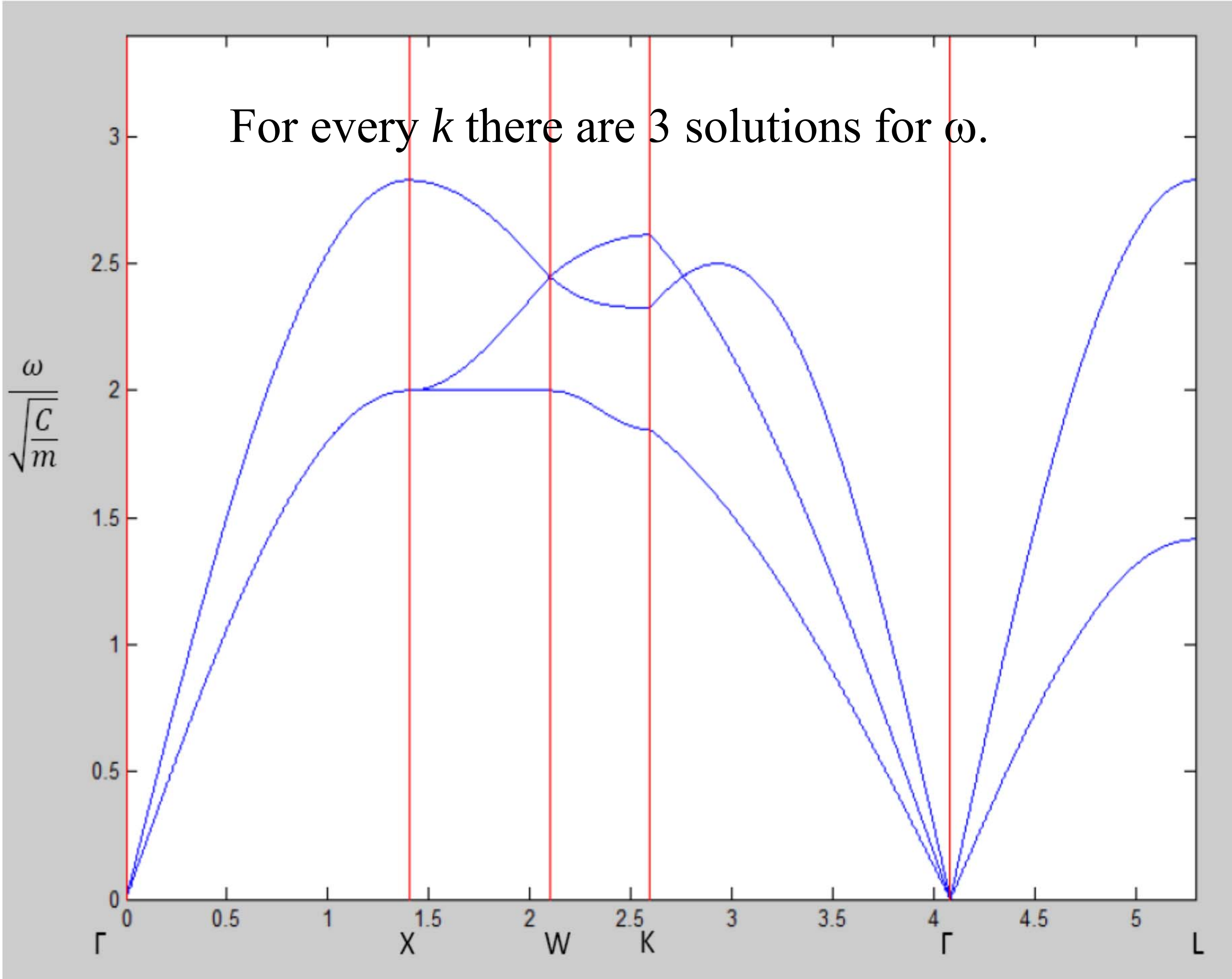
$$\vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

Substitute the eigenfunctions of T into Newton's laws.

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

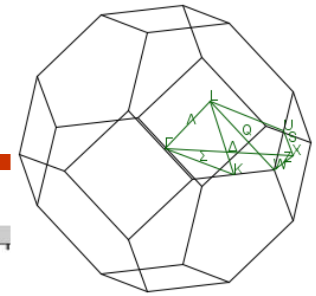
$$\begin{vmatrix} 4-\cos\left(\frac{k_xa}{2}+\frac{k_ya}{2}\right)-\cos\left(\frac{k_xa}{2}+\frac{k_za}{2}\right)-\cos\left(\frac{k_xa}{2}-\frac{k_ya}{2}\right)-\cos\left(\frac{k_xa}{2}-\frac{k_za}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_xa}{2}+\frac{k_ya}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_ya}{2}\right)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

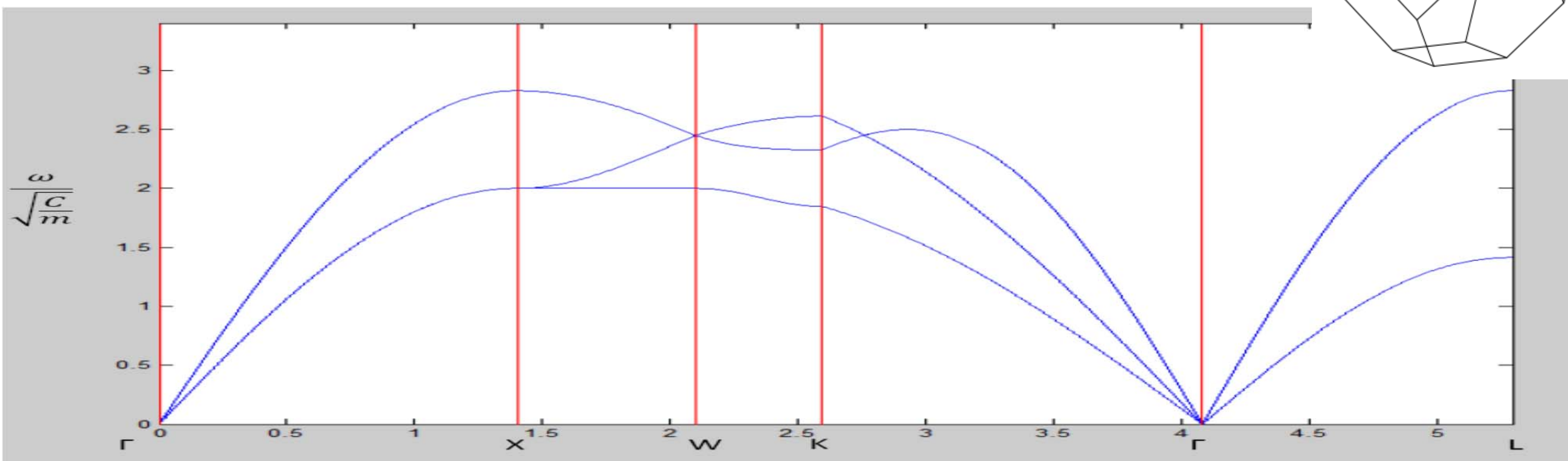
http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/fcc/fcc.html


For every k there are 3 solutions for ω.
ω / √(C/m)
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Γ
X
W
K
Γ
L

Phonon dispersion Au

From Springer Materials: Landholt Boernstein Database





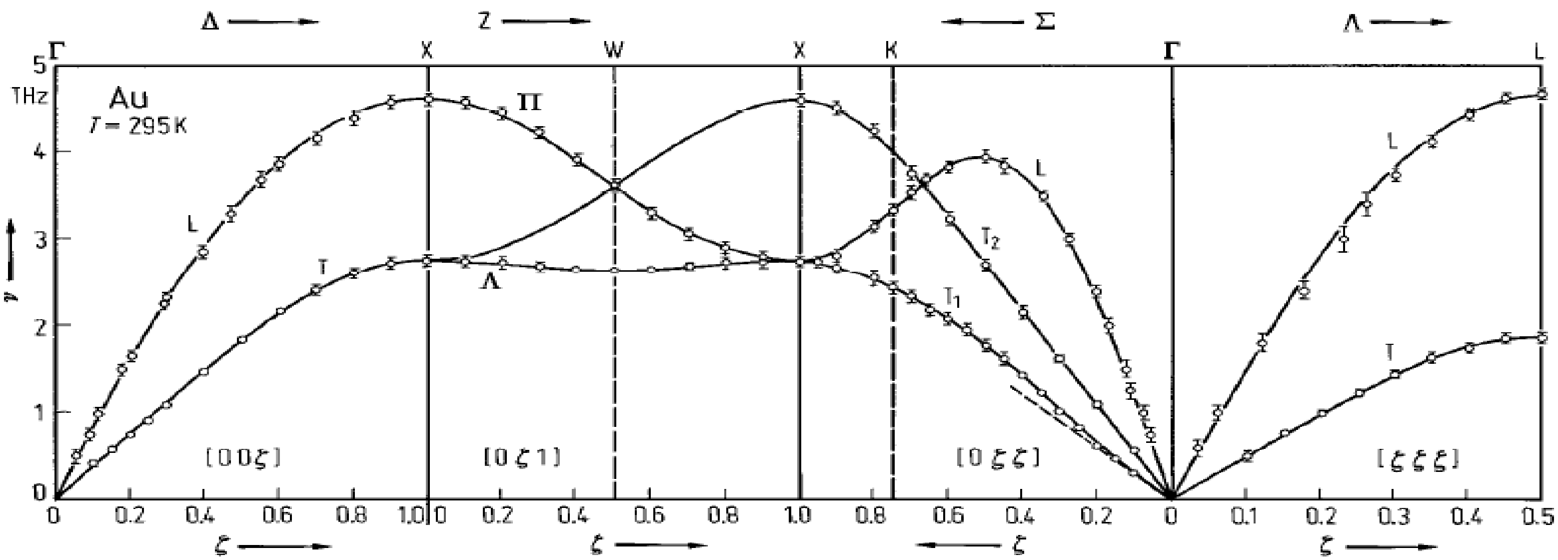
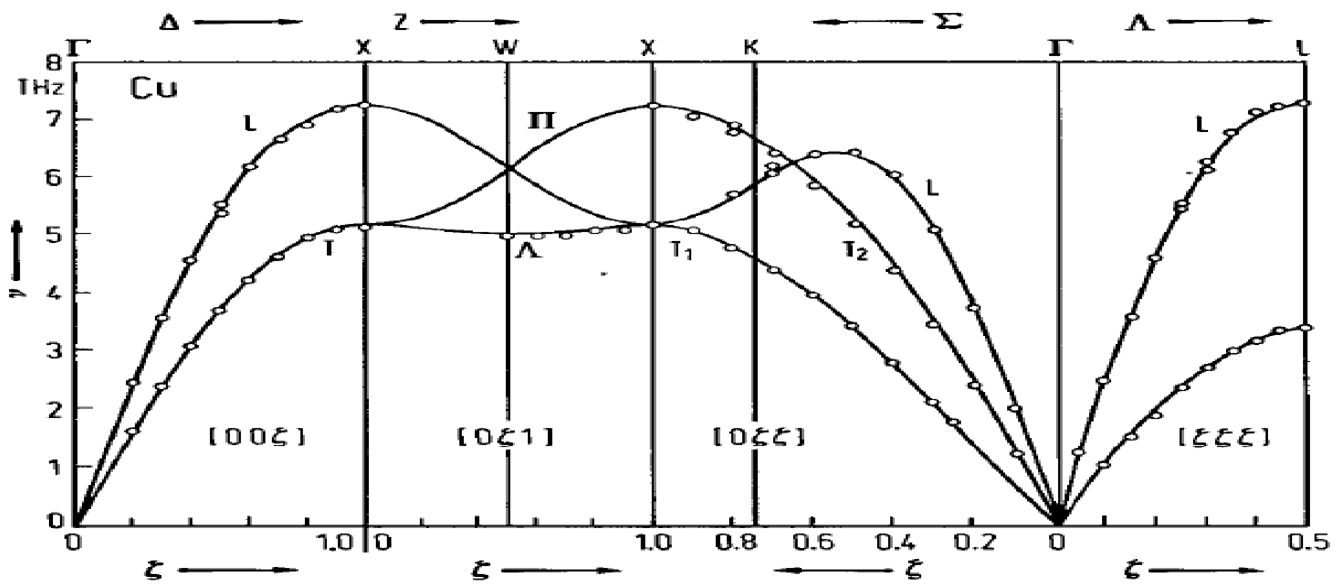


Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the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

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



Cu

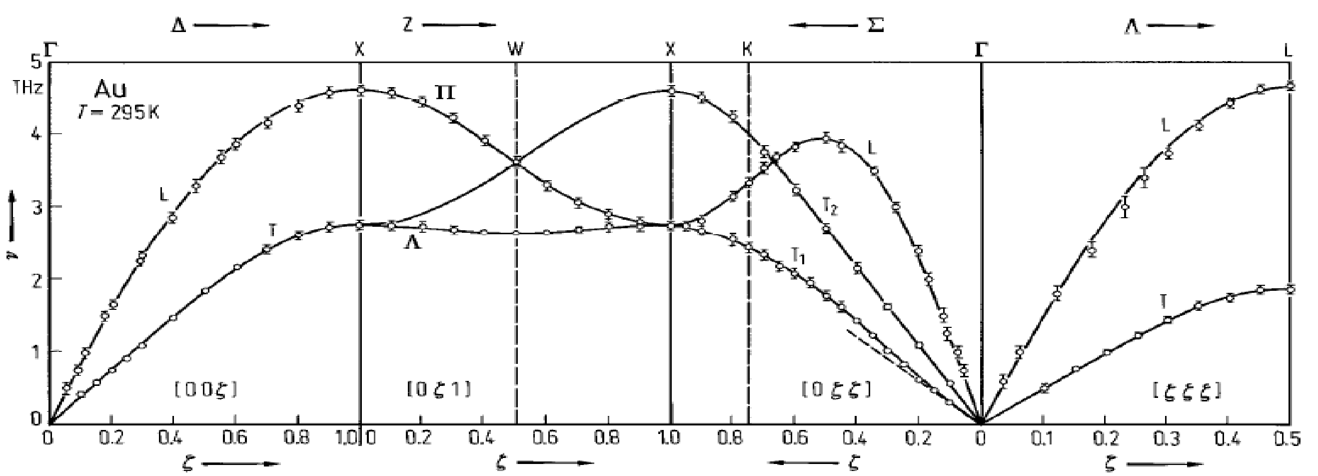
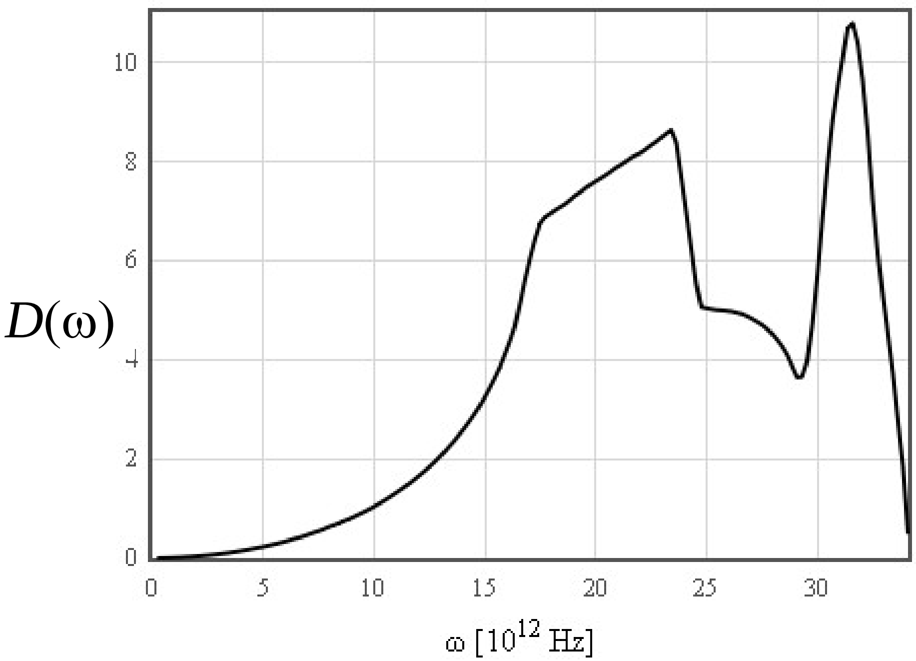


Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the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

Au

Phonon DOS fcc



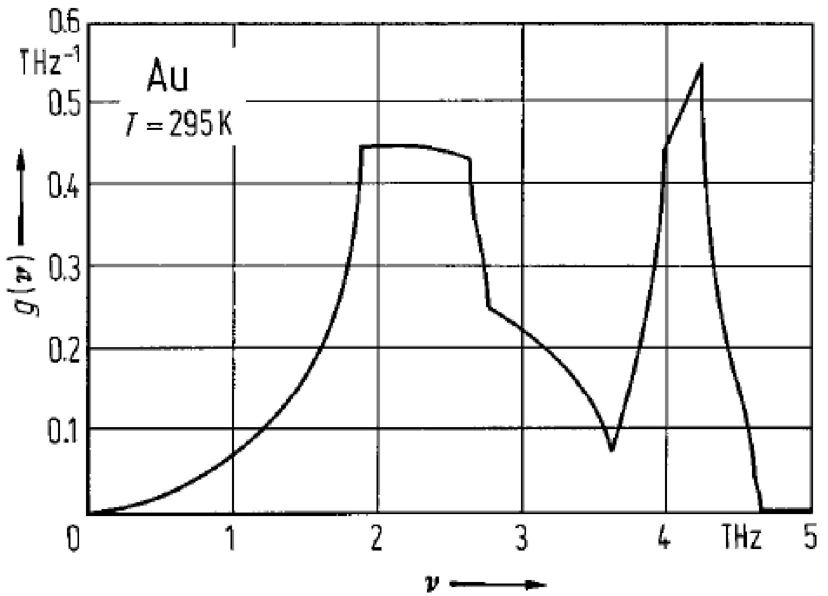
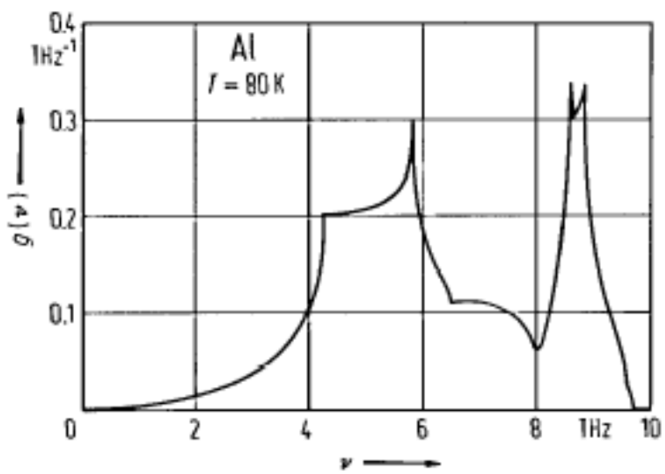
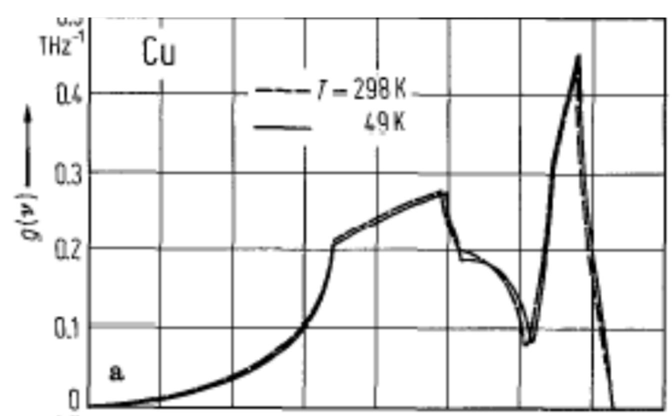


Fig. 2. Au. Frequency distribution calculated from the fourth neighbour general force constant model (M1) of Table 3 Au.





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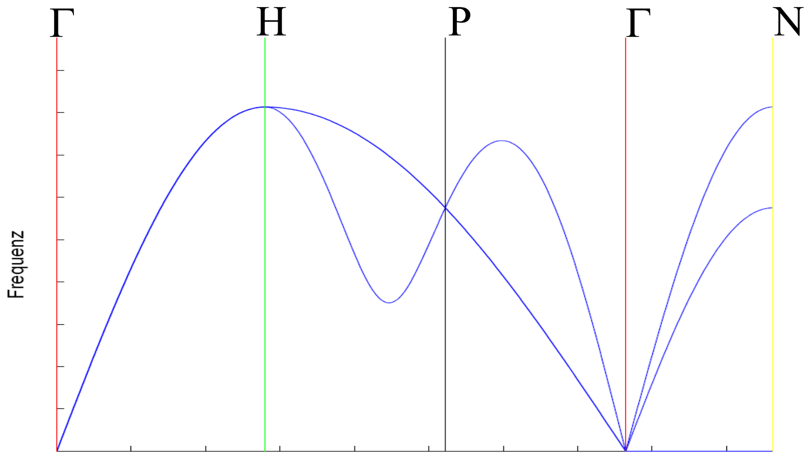
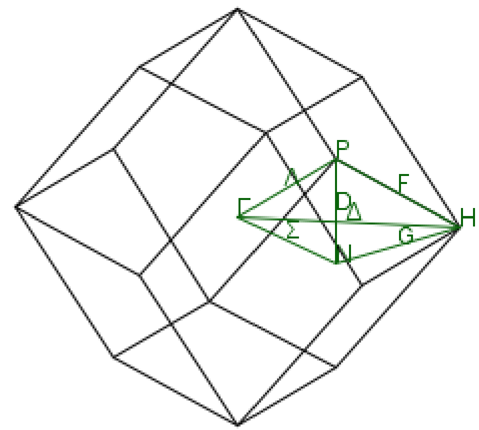
Phonon dispersion Fe





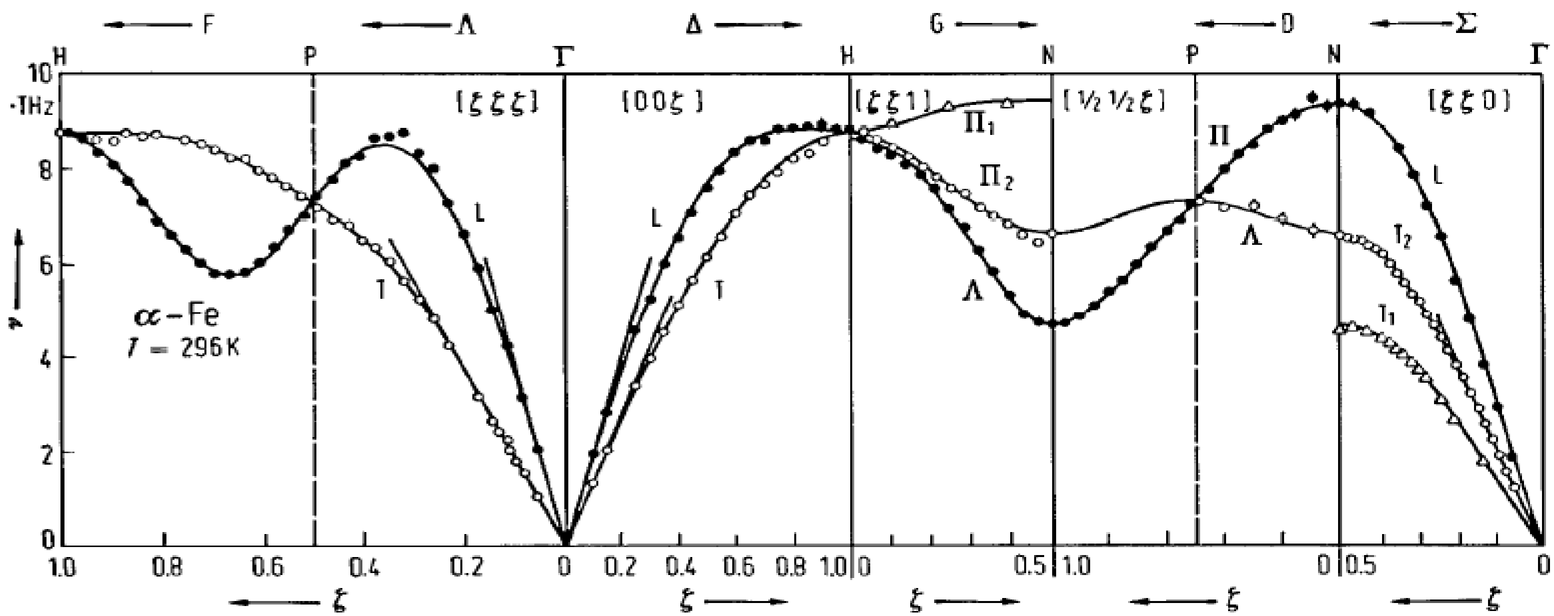


Fig. 2. Fe. Phonon dispersion curves in α-iron at 296 K. Experimental points: [68Va2]. Solid curve: fifth neighbour Born-von Karman model (Table 3 Fe [68Va2]).

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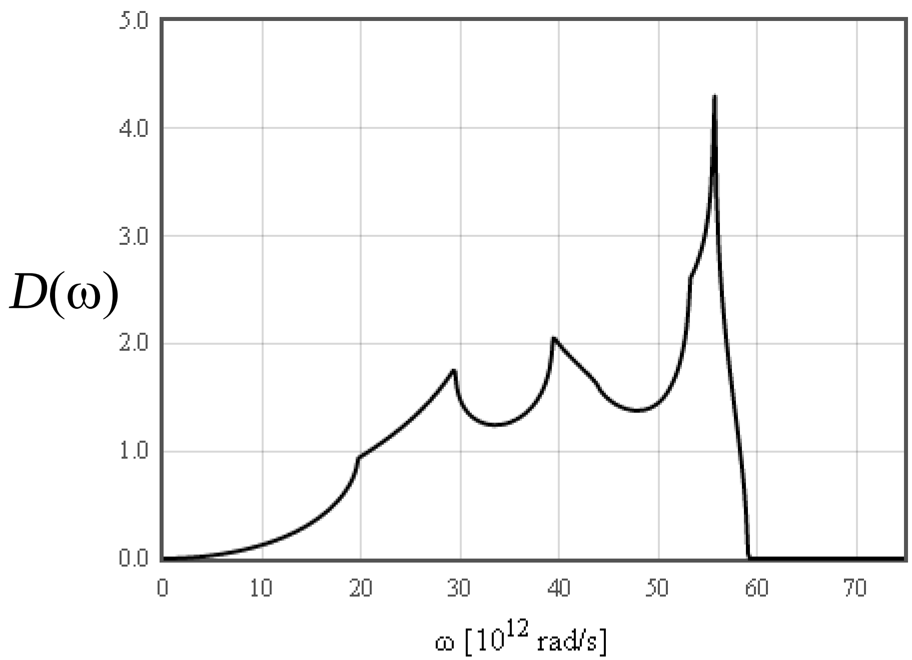
Phonon DOS Fe



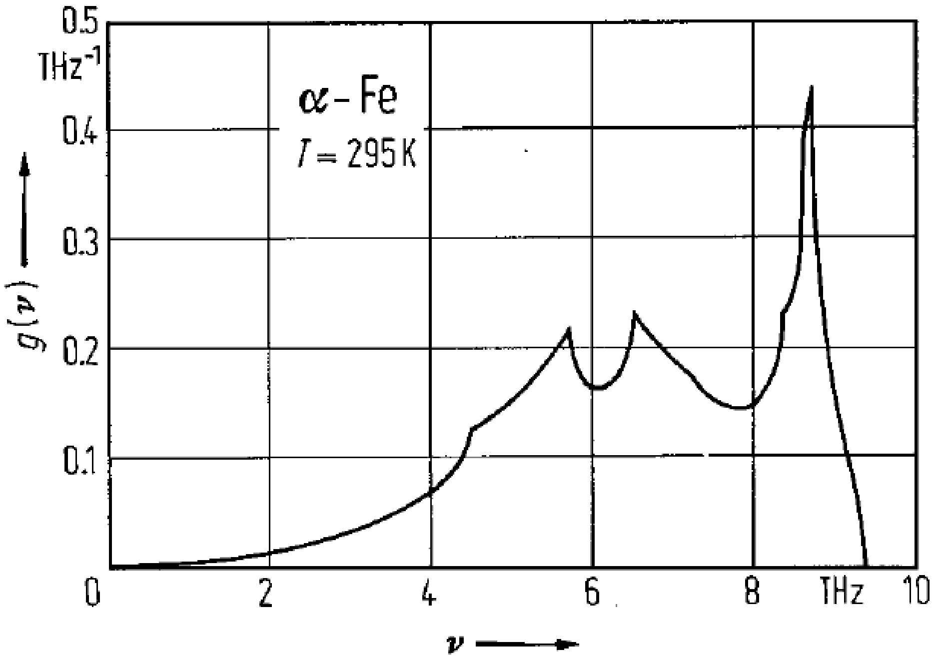


Fig. 3. Fe. Frequency spectrum of α-iron at 295 K calculated from the Born-von Karman force constants of Table 3 Fe [67Mi1].

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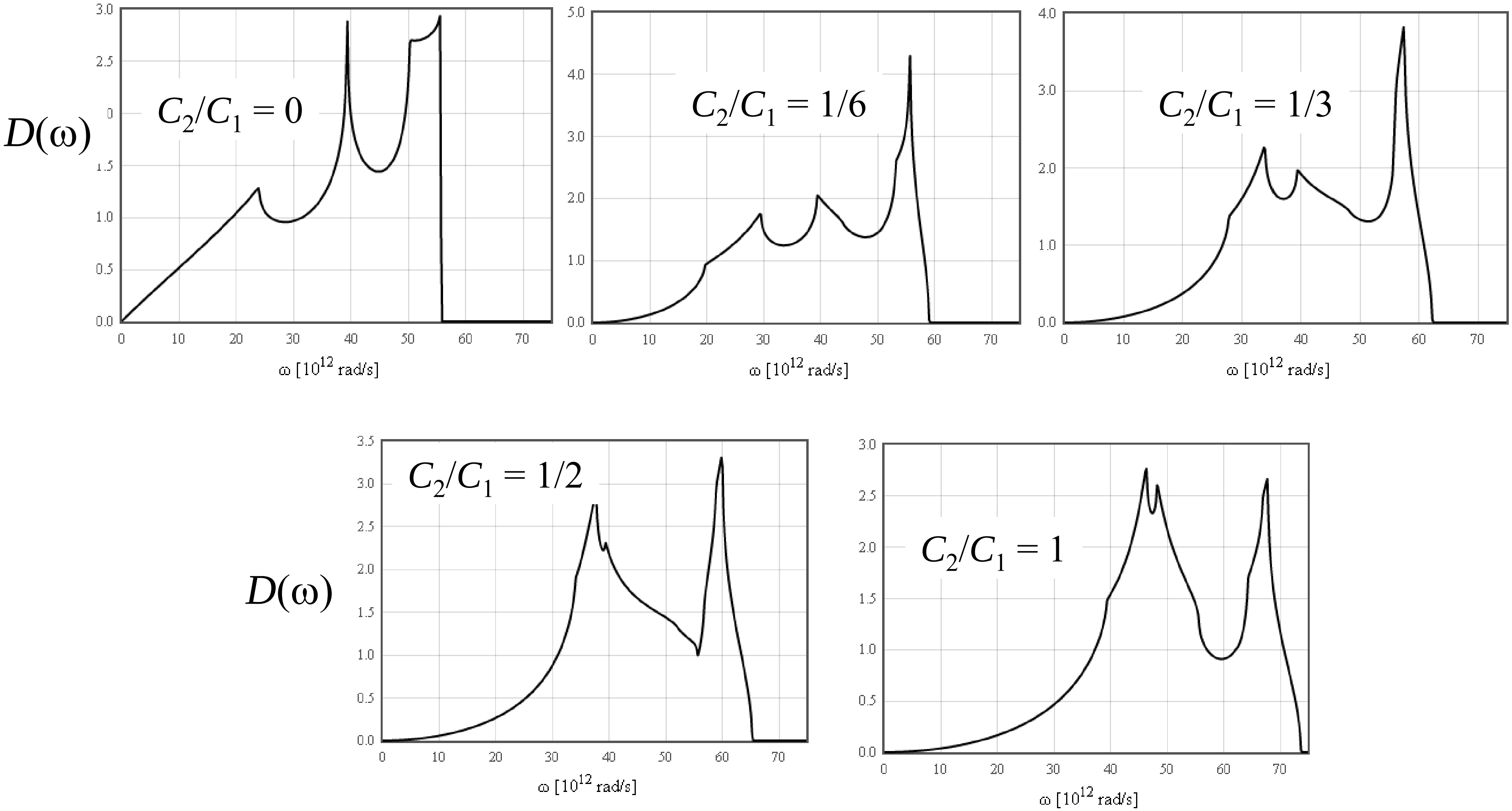
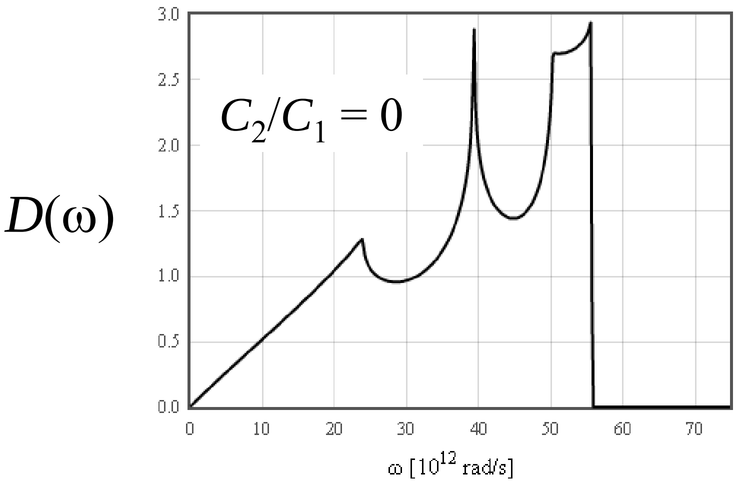
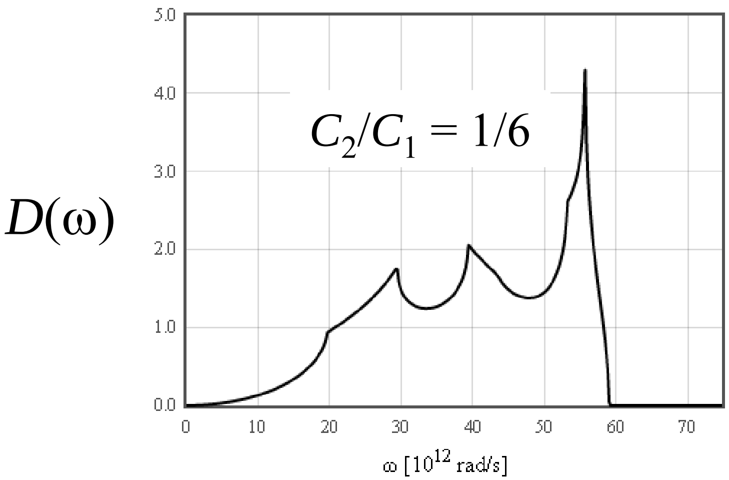
Next nearest neighbors (bcc)



The normal modes remain the same (the translational symmetry is the same).

Phonon DOS Fe





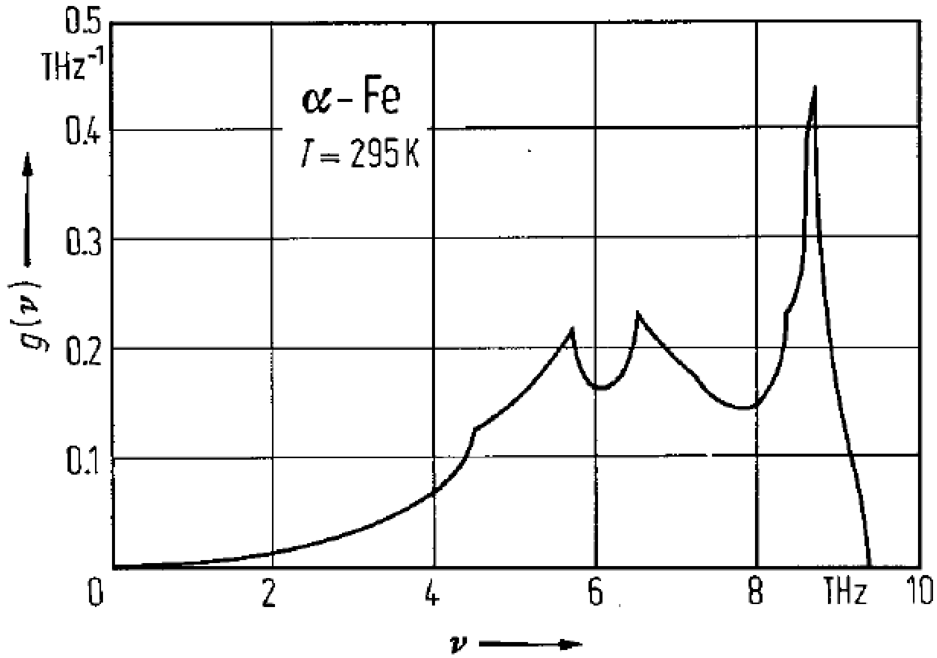


Fig. 3. Fe. Frequency spectrum of α-iron at 295 K calculated from the Born-von Karman force constants of Table 3 Fe [67Mi1].

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