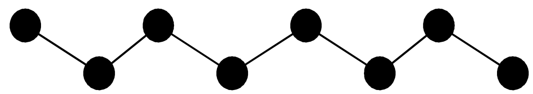
# Phonons

# Lattice vibrations / Phonons

Phonons are quantum particles of sound

The simplest model for lattice vibrations is atoms connected by linear springs

There is a shortest wavelength/maximum frequency



Find the normal mode solutions

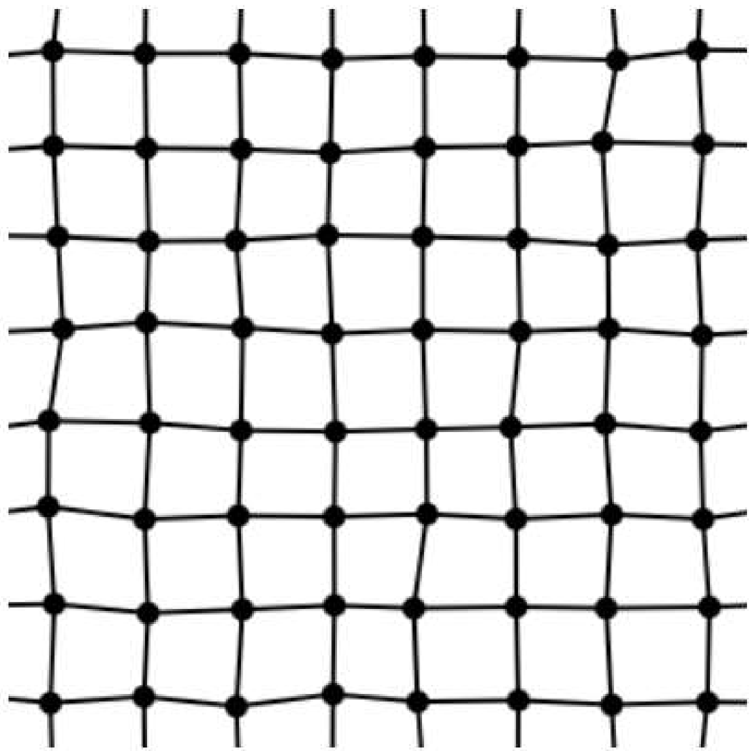
Quantize the normal modes

Find the phonon density of states

Calculate the thermodynamic properties

# Normal Modes and Phonons

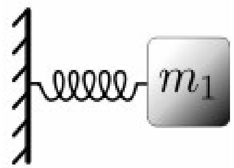
At finite temperatures, the atoms in a crystal vibrate. In the simulation below, the atoms move randomly around their equilibrium positions.



$T$ = 300 K - +

http://lampx.tugraz.at/~hadley/ss1/phonons/phonon_script.php

# Vibrations of a mass on a spring




$$m\frac{d^2x}{dt^2} = -Cx$$

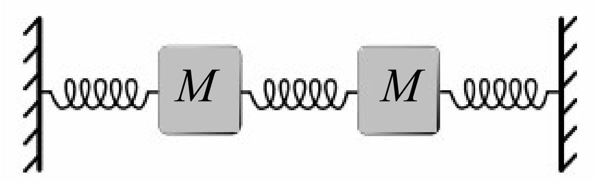
The solution has the form

$$x = A\mathrm{e}^{-i\omega t}$$

$$-\omega^2 mAe^{-i\omega t} = -CAe^{-i\omega t}$$

$$\omega = \sqrt{\frac{C}{m}}$$

# Coupled masses




Newton's law

$$M\frac{d^2x_1}{dt^2} = -Cx_1 + C\left(x_2 - x_1\right) \qquad M\frac{d^2x_2}{dt^2} = -Cx_2 + C\left(x_1 - x_2\right)$$

assume harmonic solutions

$$x_1(t) = A_1\exp(i\omega t) \qquad x_2(t) = A_2\exp(i\omega t)$$

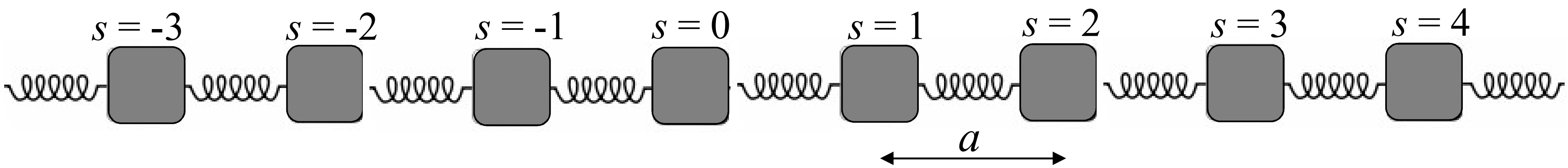
$$-\omega^2 MA_1e^{i\omega t} = -2CA_1e^{i\omega t} + CA_2e^{i\omega t}$$
$$-\omega^2 MA_2e^{i\omega t} = -2CA_2e^{i\omega t} + CA_1e^{i\omega t}$$

$$-\omega^2 M\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} -2C & C \\ C & -2C \end{bmatrix}\begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$$

Find the eigenvectors of this matrix

The masses oscillate with the same frequency but different phases

# 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 $u_s = A_s e^{-i\omega t}$

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

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

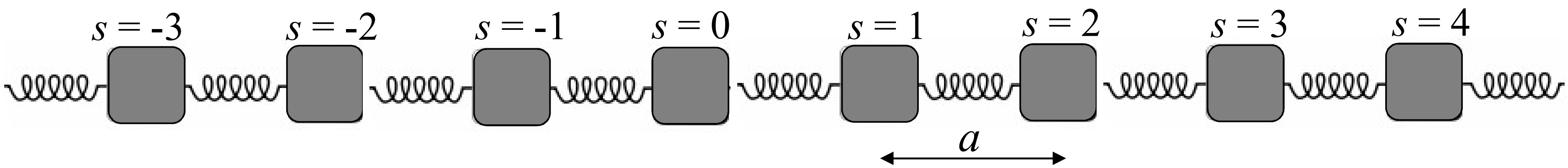
# Eigen vectors of the translation operator

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

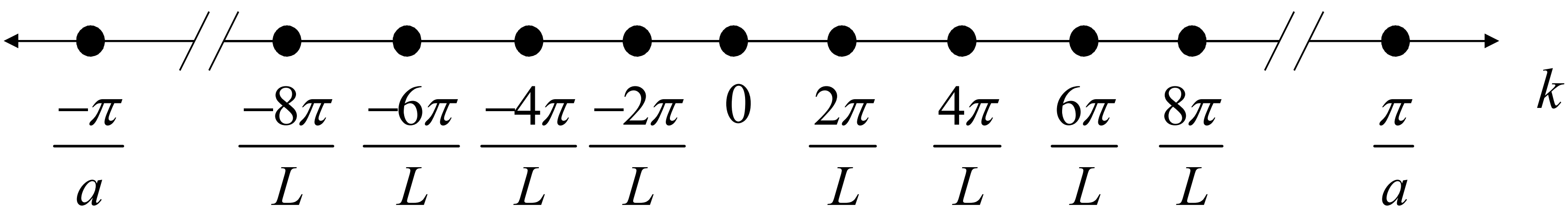
$$\begin{bmatrix} 1 \\ e^{i2\pi j/N} \\ e^{i4\pi j/N} \\ e^{i4\pi j/N} \\ \vdots \\ e^{i2\pi(N-1)j/N} \end{bmatrix} \qquad j = 1, \cdots, N$$

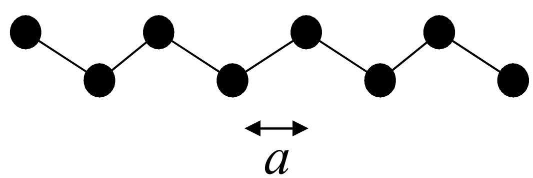
$$\begin{bmatrix} 1 \\ e^{ika} \\ e^{i2ka} \\ e^{i3ka} \\ \vdots \\ e^{-ika} \end{bmatrix} \qquad k = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \cdots$$

# Linear Chain

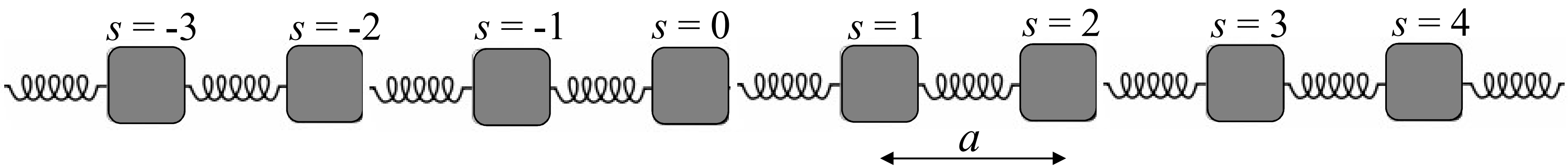



solution: $u_s = A_k e^{i(ksa-\omega t)} = A_k e^{iksa} e^{-i\omega t}$



# Normal modes are eigen functions of T



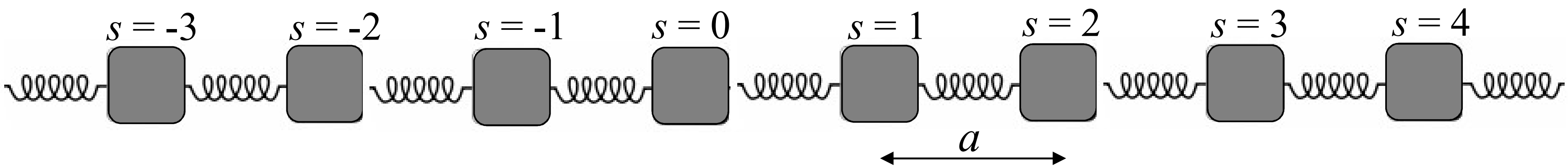

solutions are eigenfunctions of the translation operator

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

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

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

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

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

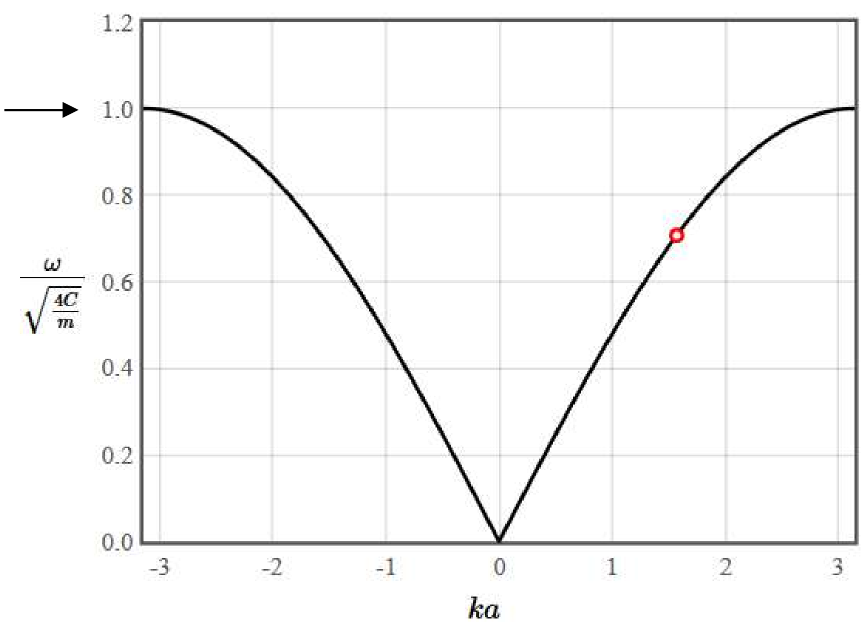
$$\omega^2 m = 2C(1-\cos(ka))$$

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

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

# Linear Chain - dispersion relation

Max. freq.





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

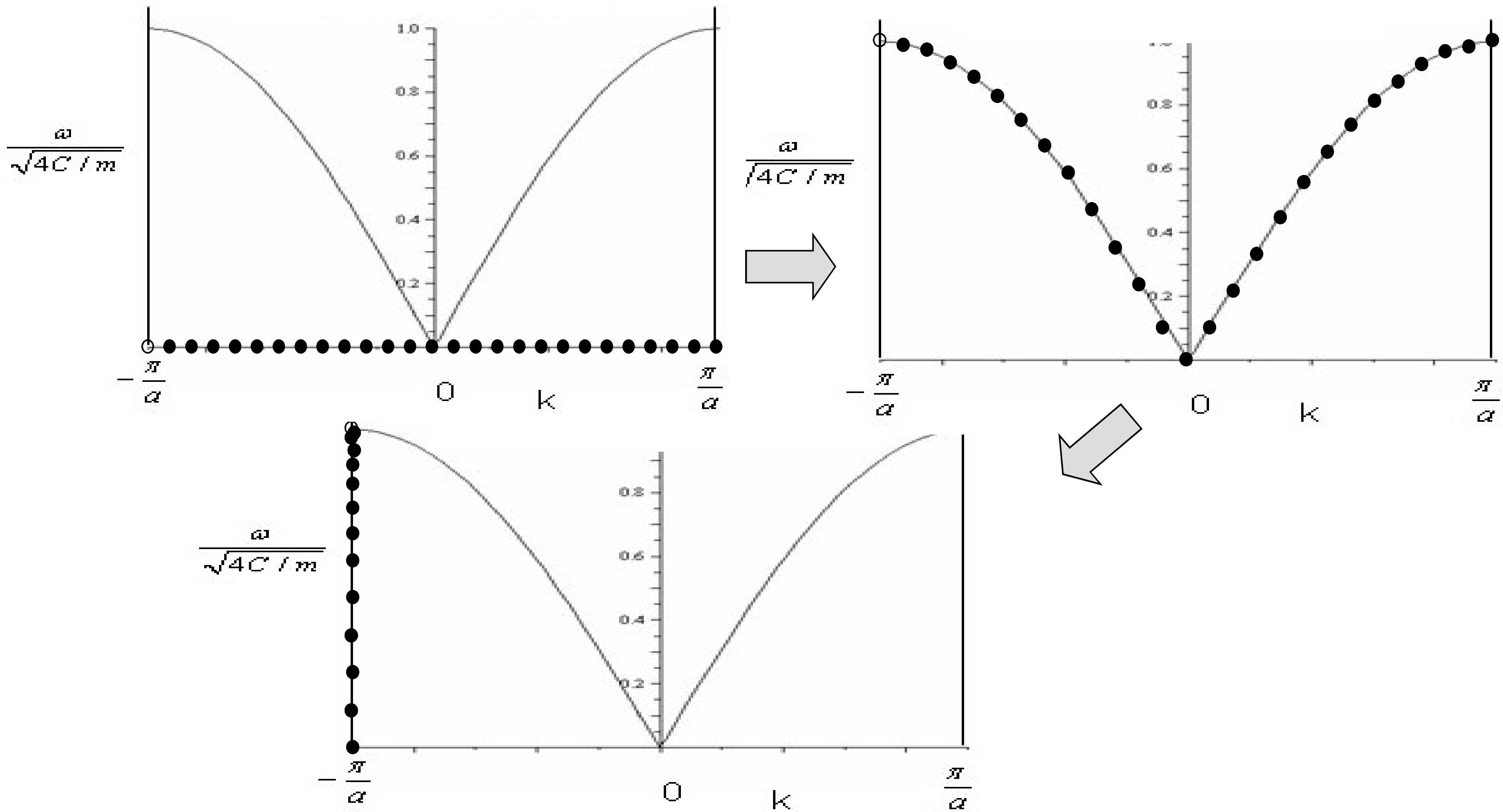
$$u_s = A_k e^{i(ksa-\omega t)}$$

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

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

# Linear Chain - density of states

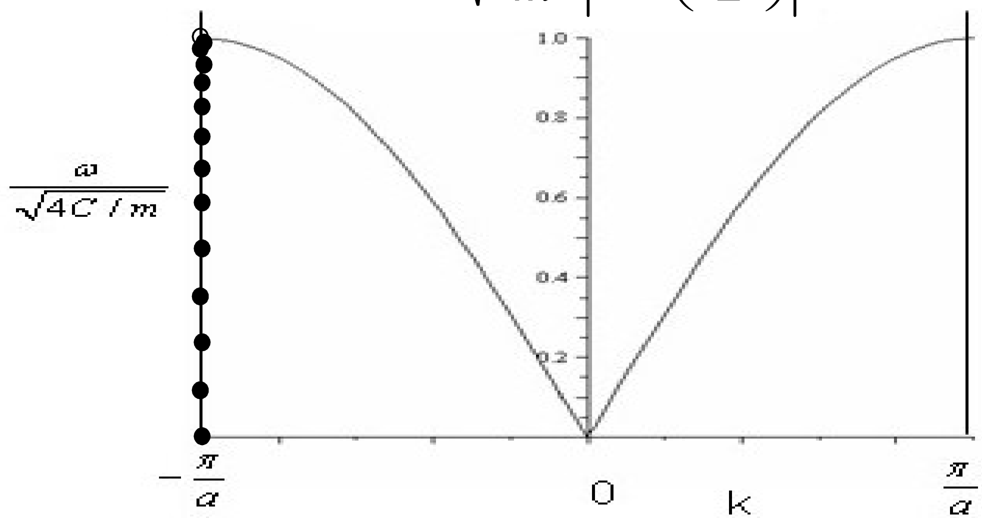
Determine the density of states numerically $\omega = \sqrt{\frac{4C}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$



# 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

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

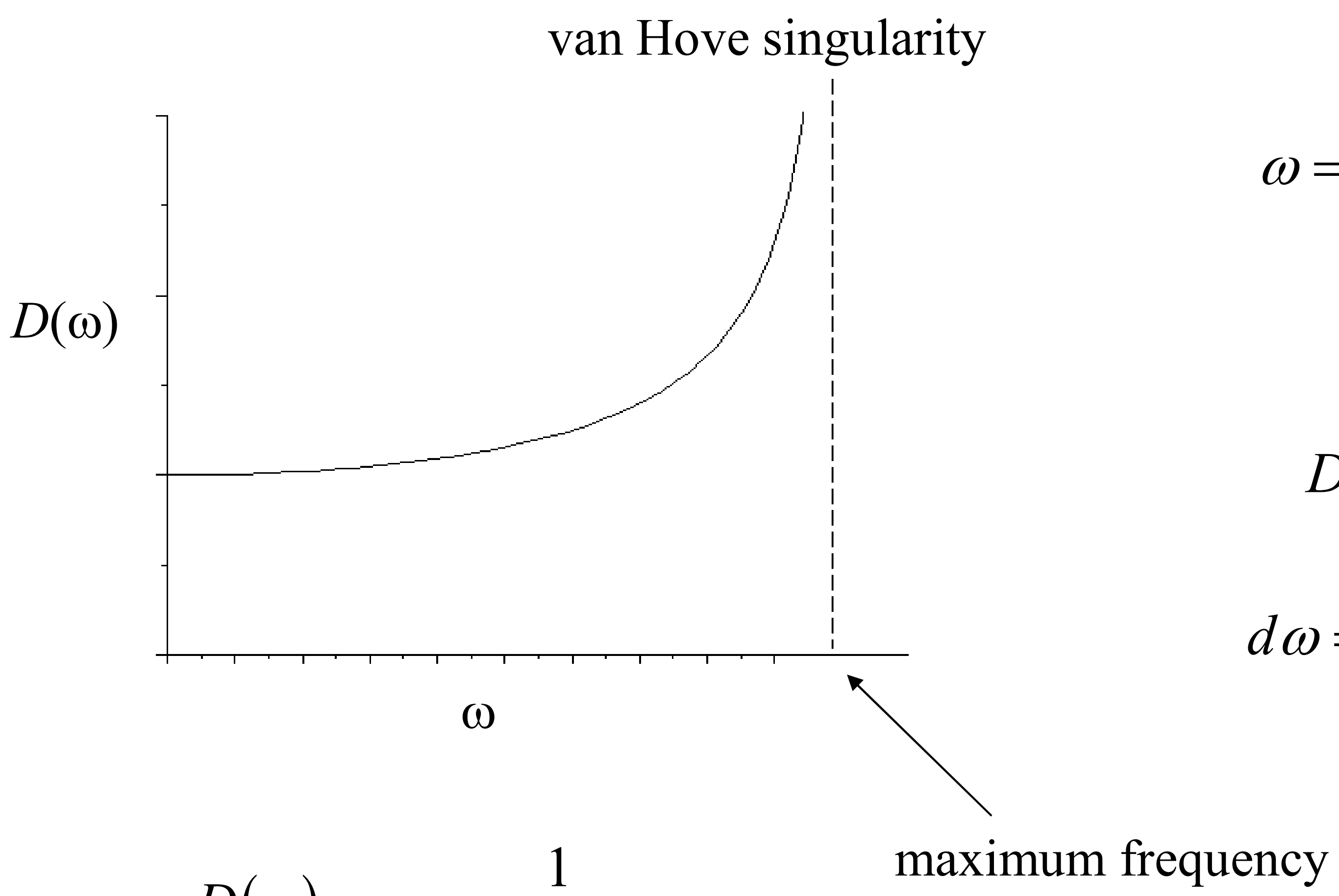
$$D(k) = \frac{1}{\pi}$$

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

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

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

# density of states




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

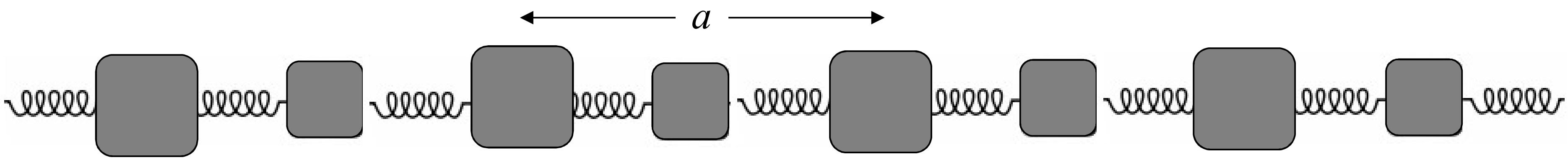
$$D(k) = \frac{1}{\pi}$$

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

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

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

# 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

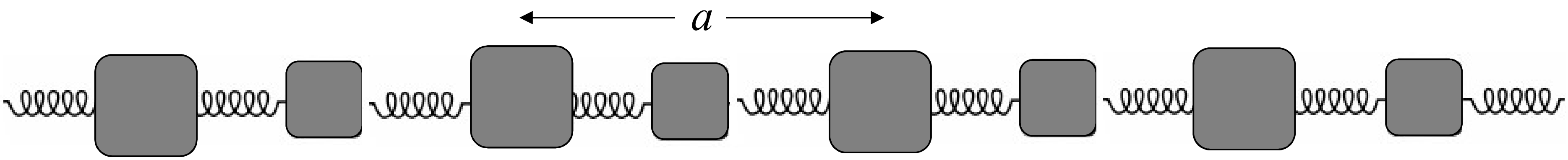
$$u_s = u_k e^{i(ksa - \omega t)}$$

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

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

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

# Linear chain $M_1$ and $M_2$




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

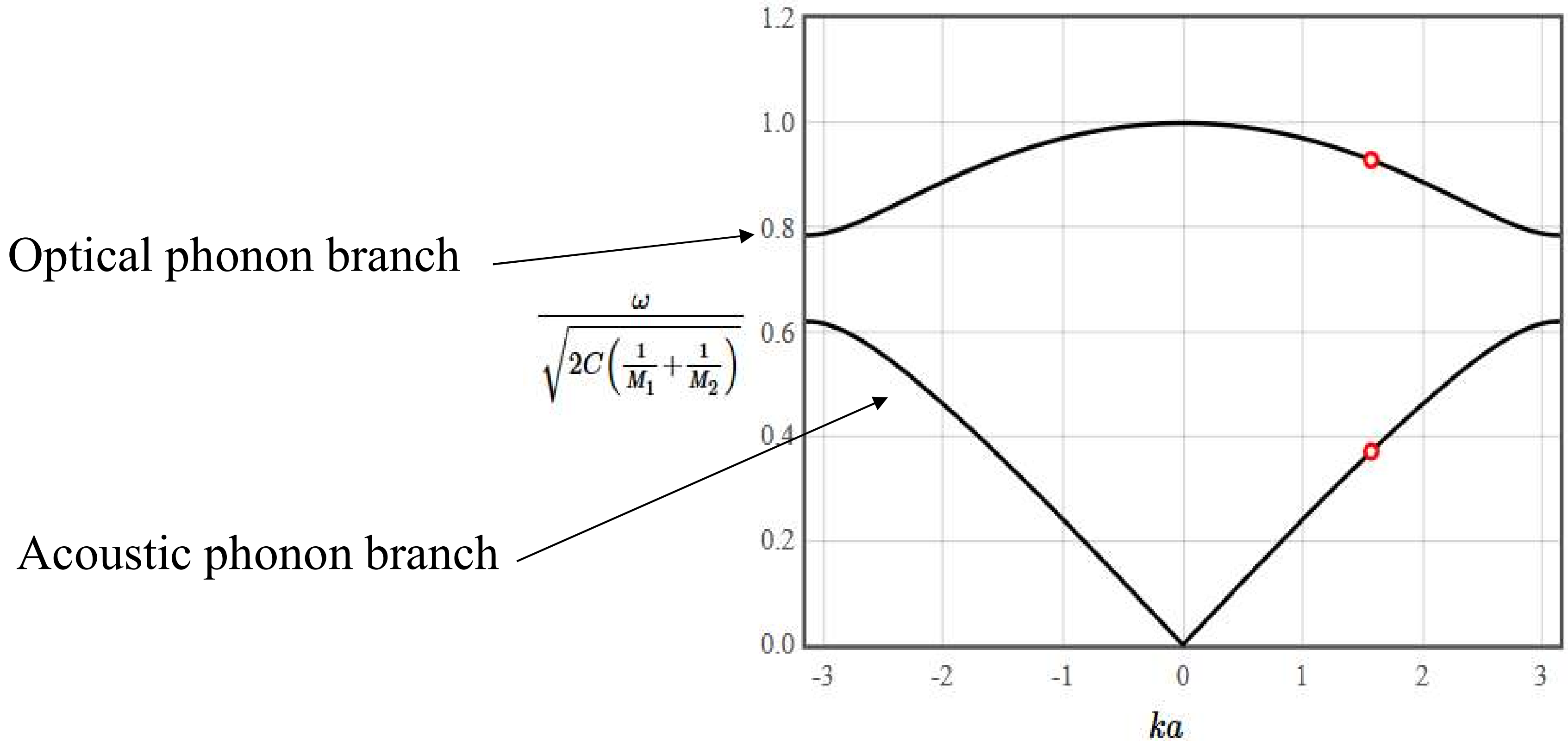
$$-\omega^2 M_2 v_k = C u_k (1+\exp(ika)) - 2Cv_k$$

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

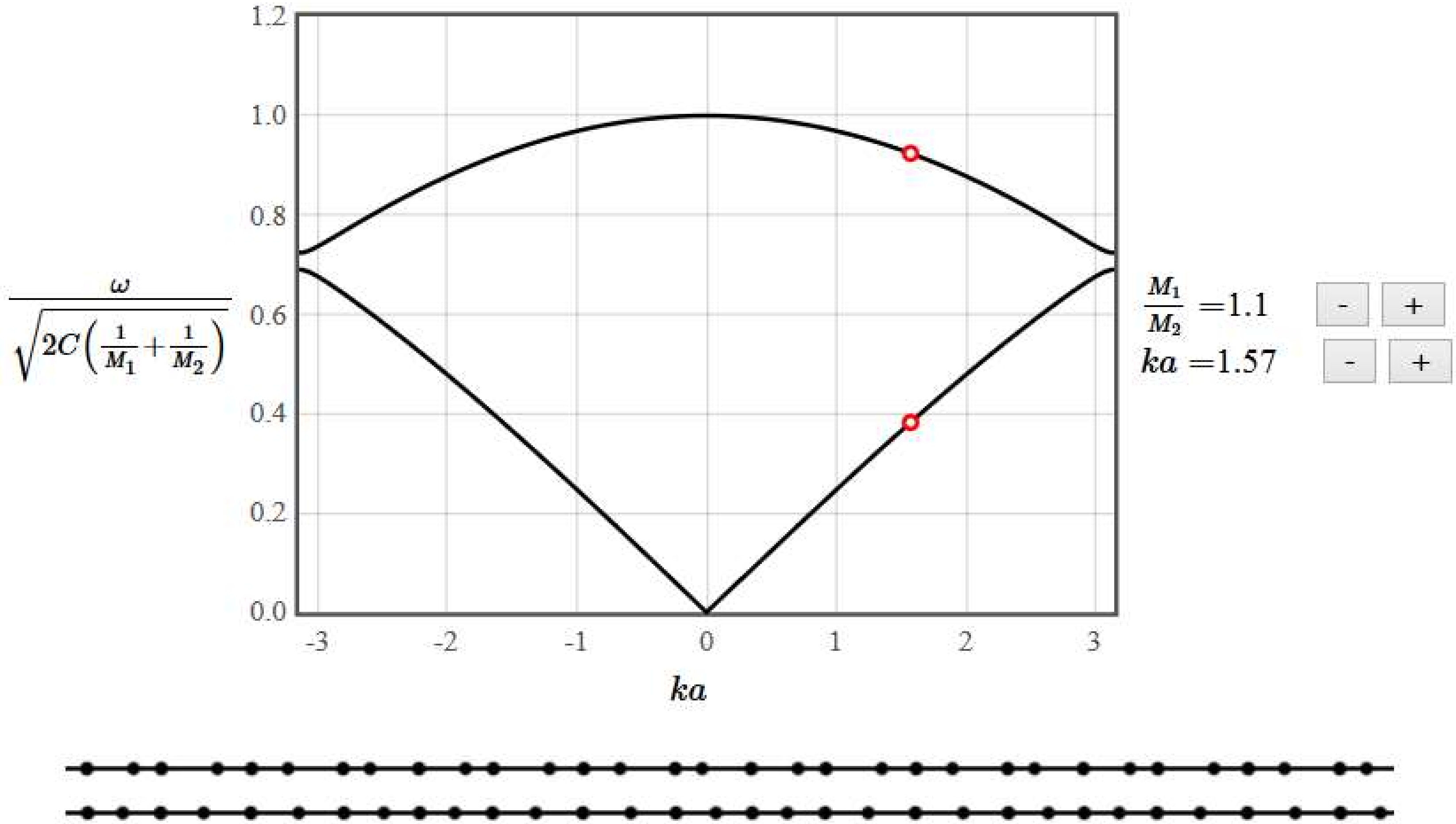
$$M_1 M_2 \omega^4 - 2C\left(M_1 + M_2\right)\omega^2 + 2C^2\left(1-\cos(ka)\right) = 0$$

# dispersion relation

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

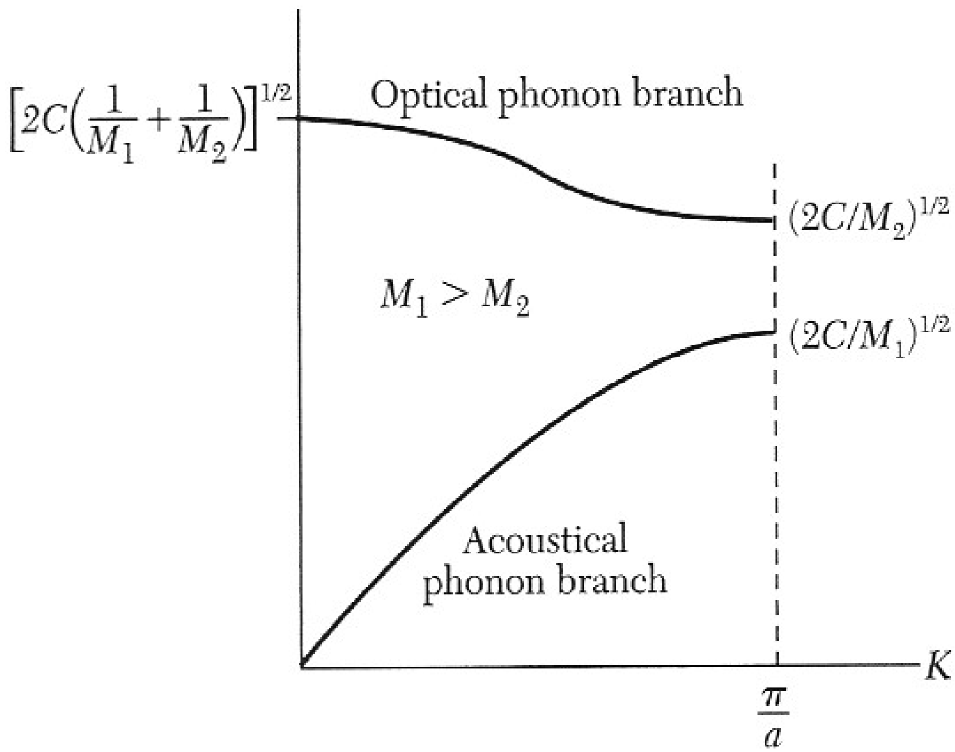


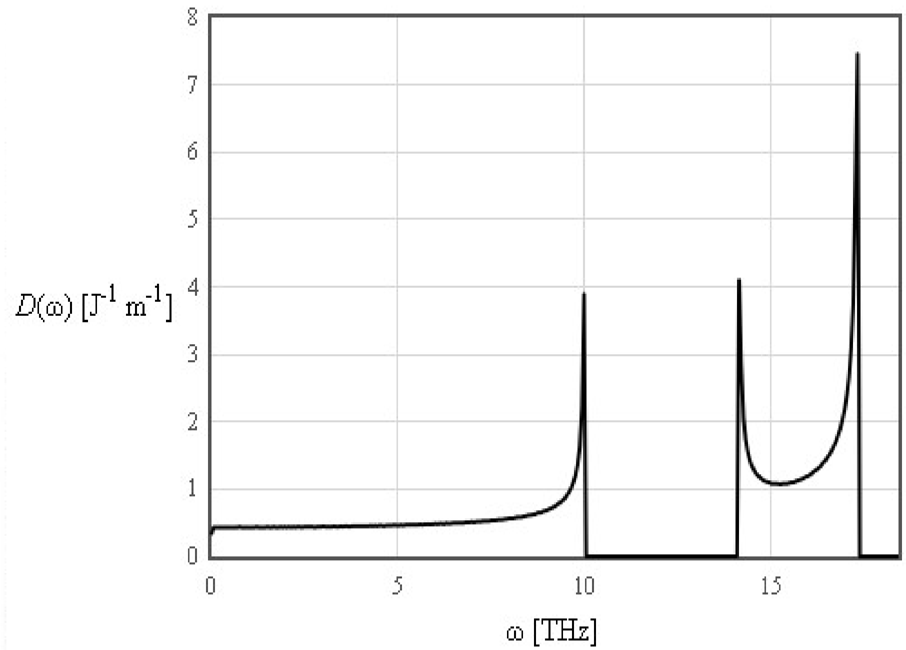
# normal modes




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

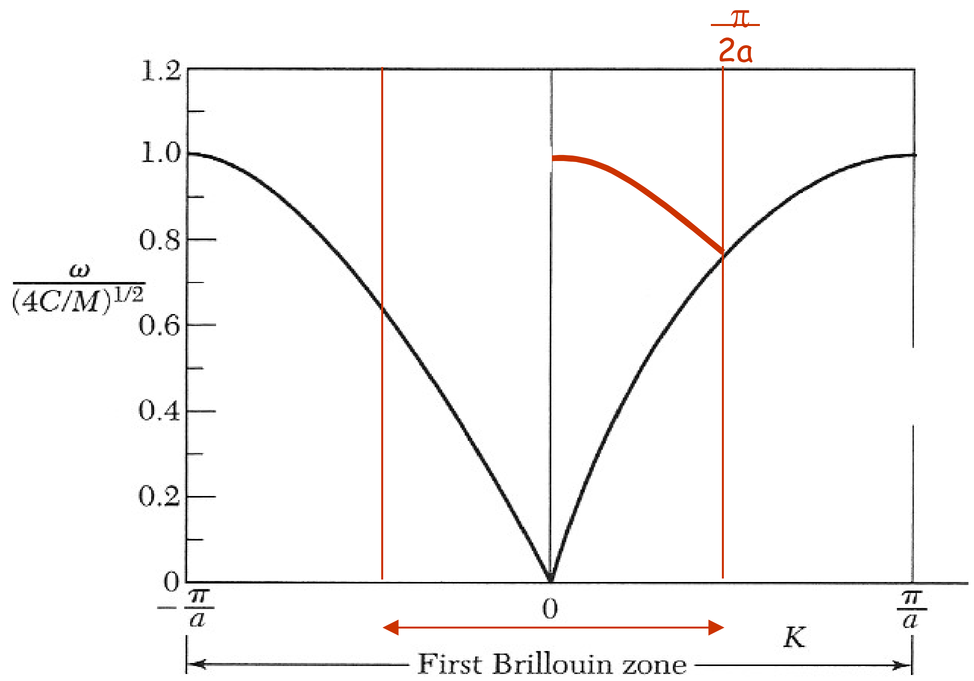
# density of states

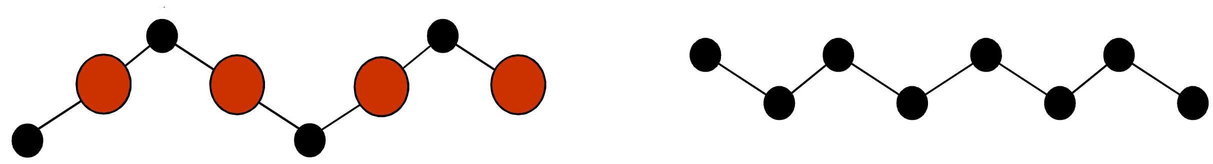


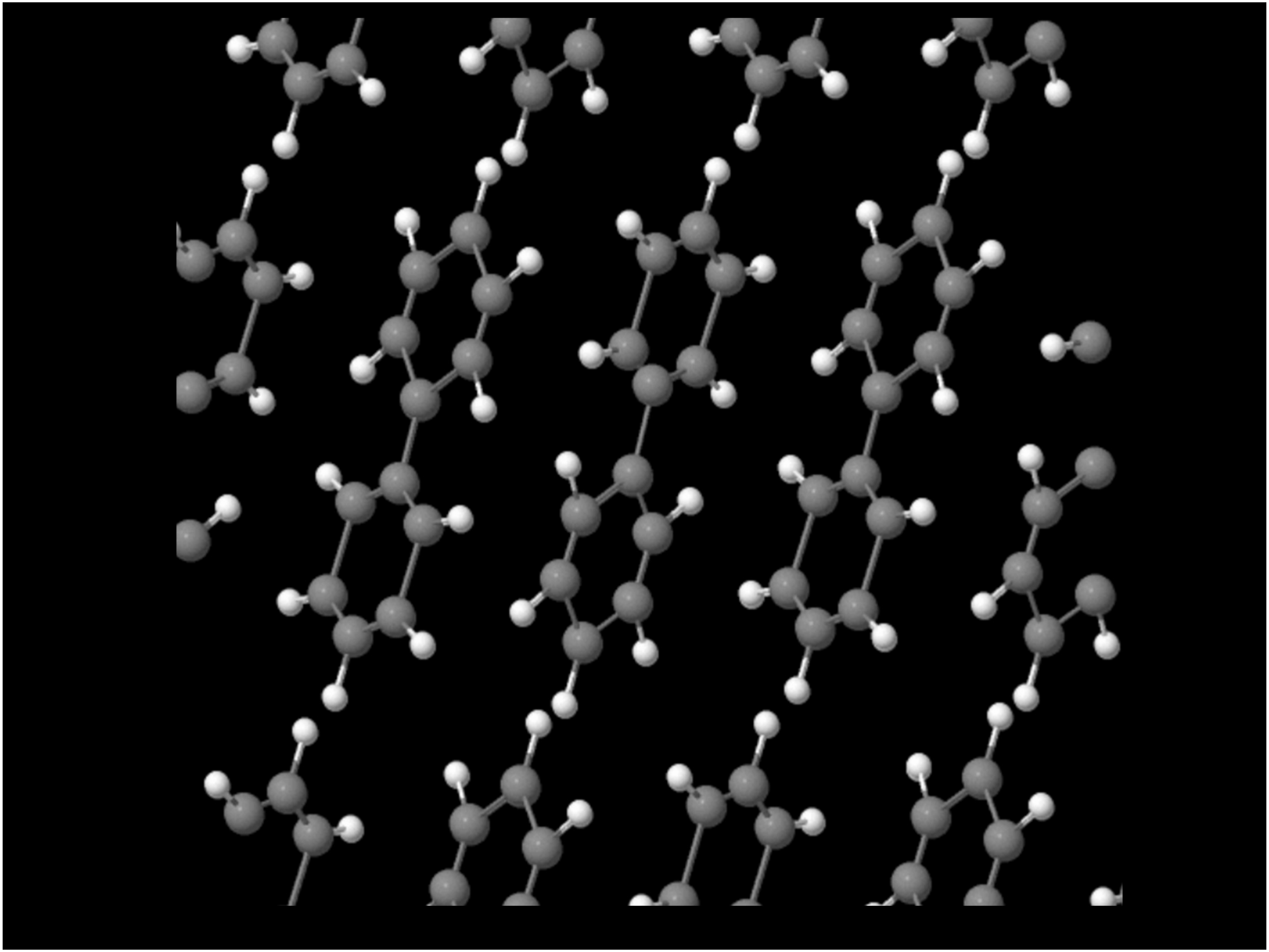

$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2 ka}{M_1 M_2}}$$

# Linear chain $M_1$ and $M_2$

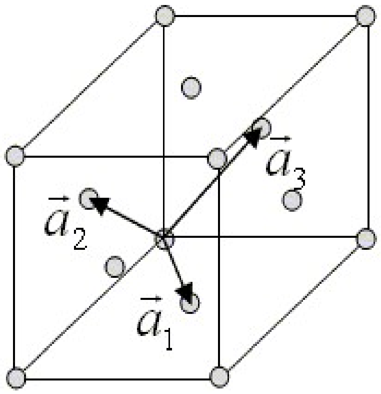


The branches of the dispersion curves can be translated by a reciprocal lattice vector $\vec{G}$.



# fcc




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

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

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

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

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

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

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

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

# Normal modes are eigenfunctions of T

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

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

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

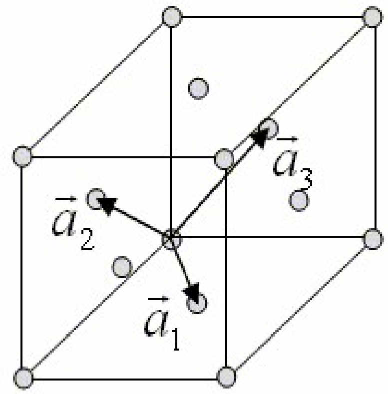
These are eigenfunctions of T.

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

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

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

# 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.