Diffraction Phonons

Particle beams

Particles moving in vacuum have the following energy-momentum relation.

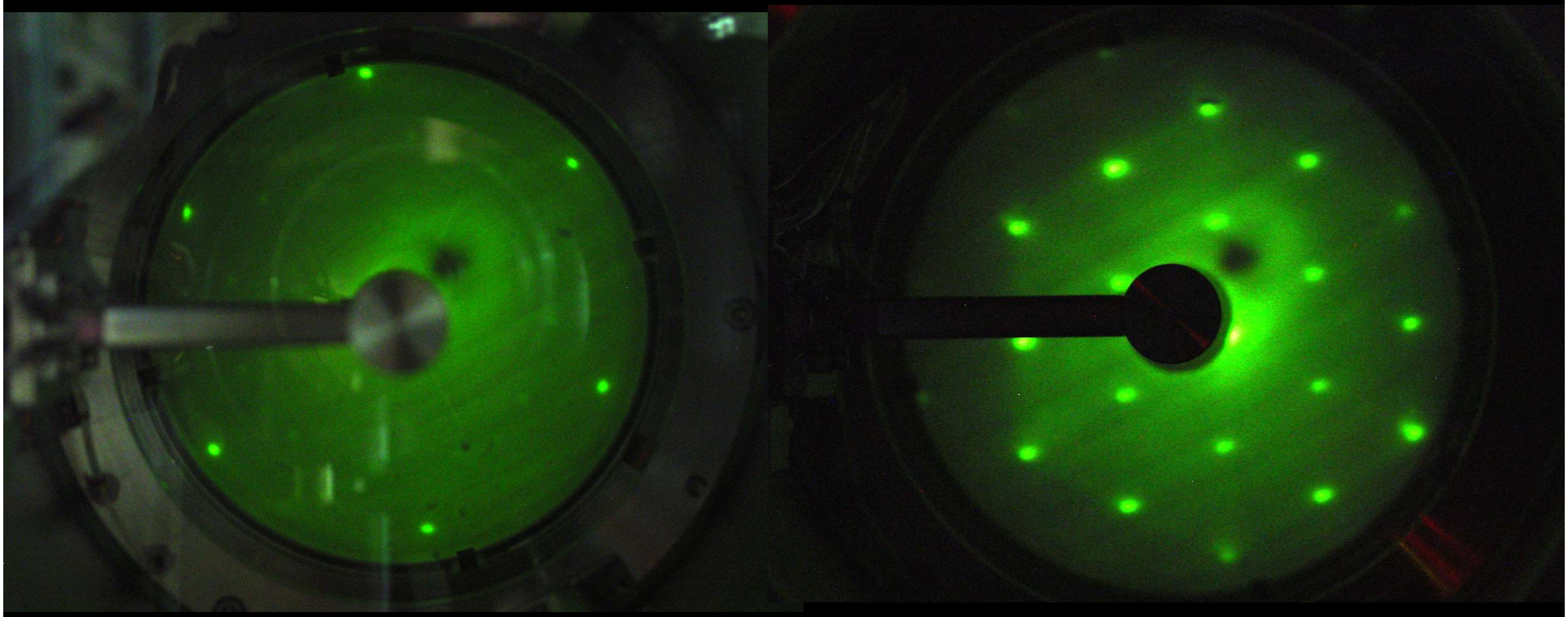
$$E = \tfrac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2}$$

If λ is much smaller than the distance between atoms, you can generate a diffraction pattern.

LEED

Low Energy Electron Diffraction

$100\ \text{V} \rightarrow k \sim 5 \times 10^{10}\ \text{m}^{-1}$



Clean Pd (111)

Pd (111) + 0.3 ML VO_x

LEED is surface sensitive

LEED

http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/atomicformfactors/LEED.php

Energy of the electron beam: 100 [eV]

Primitive lattice vectors:

$\vec{a}_1 =$ 4.12E-10 $\hat{x} +$ 0 $\hat{y}$ [m]

$\vec{a}_2 =$ 0 $\hat{x} +$ 4.12E-10 $\hat{y}$ [m]

Basis:

The positions of the atoms are given in fractional coodinates between -1 and 1.

Cs	0	$\vec{a}_1 +$	0	$\vec{a}_2$	
Cl	0.5	$\vec{a}_1 +$	0.5	$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	

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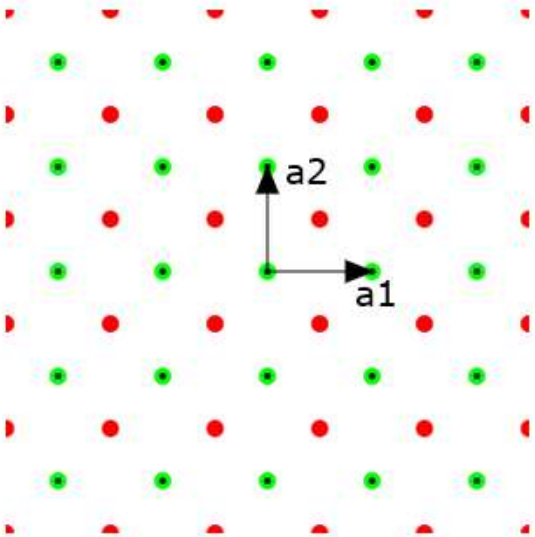
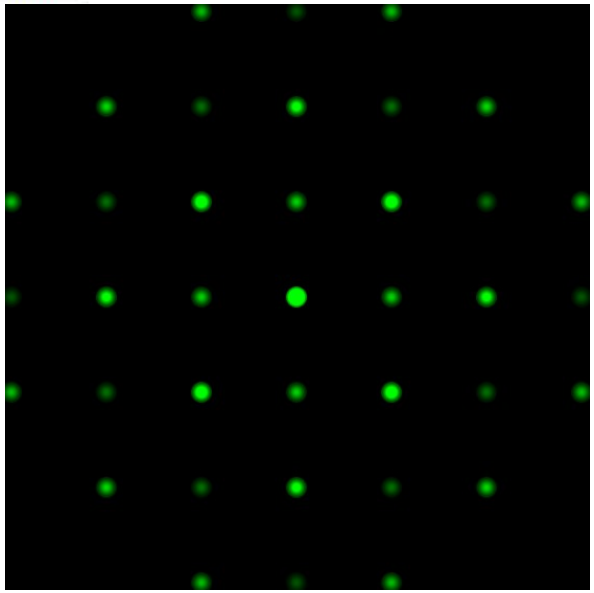
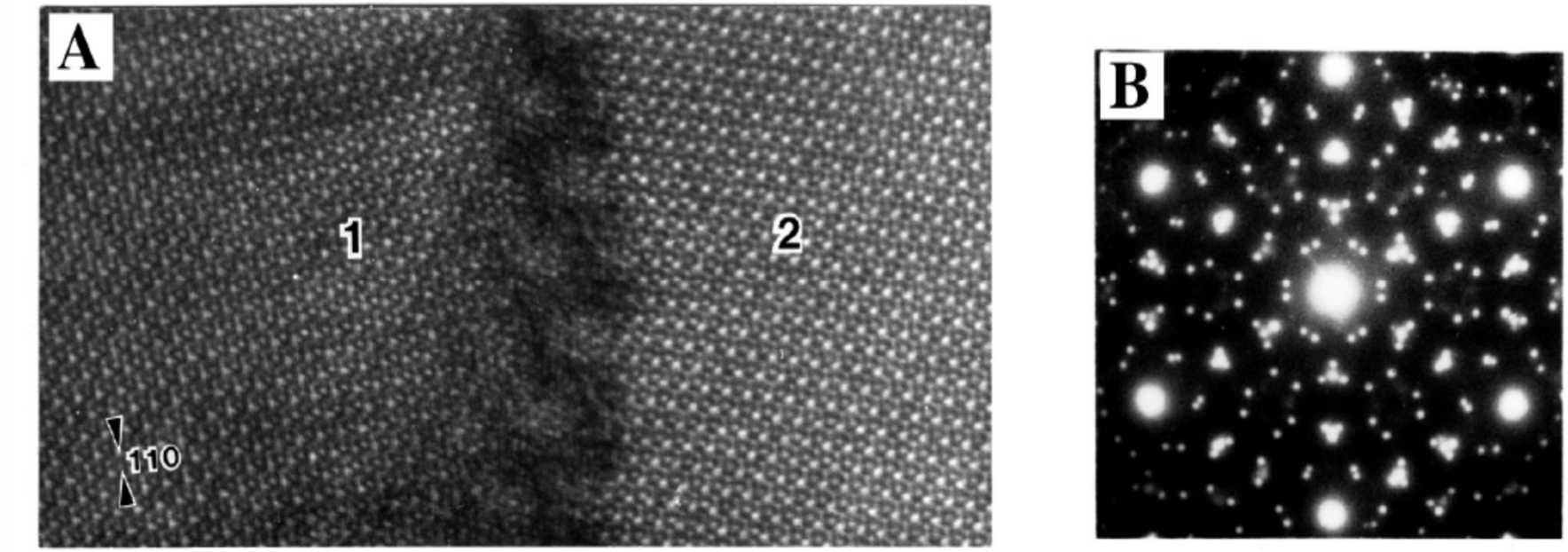




Electron diffraction in a TEM



The wavelength of the electrons is typically much smaller than the lattice spacing. The diffraction peaks in the plane perpendicular to k are observed.

Electron diffraction

In electron diffraction, the intensity of a diffraction peak at reciprocal lattice vector $\vec{G}$ is the square of the structure factor, $n_{\vec{G}}$.

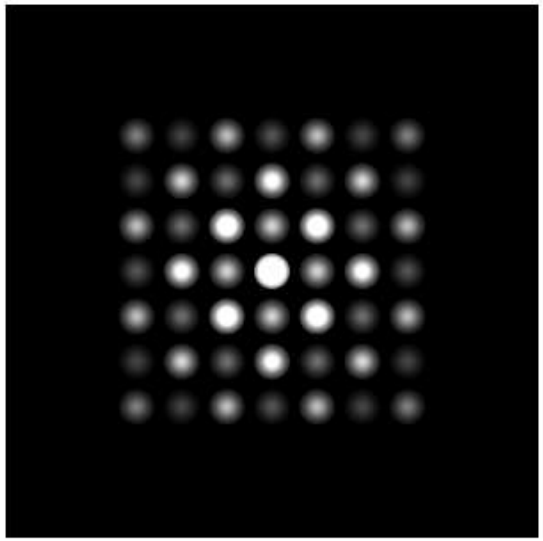
$$n_{\vec{G}} = \frac{1}{V}\sum_j f_j\left(\vec{G}\right)e^{-i\vec{G}\cdot\vec{r}_j} = \frac{1}{V}\sum_j f_j\left(\vec{G}\right)\left(\cos\left(\vec{G}\cdot\vec{r}_j\right) - i\sin\left(\vec{G}\cdot\vec{r}_j\right)\right)$$

Here V is the volume of the primitive unit cell, j sums over the atoms in the basis, $\vec{r}_j$ are the positions of the atoms in the basis, and $f_j\left(\vec{G}\right)$ are the electron atomic form factors evaluated at $\vec{G}$.

The form below calculates the electron structure factors based on this formula. The crystal structure is specified by providing the primitive lattice vectors and the positions of the atoms in the basis. A basis of up to five atoms can be calculated. The script first calculates the primitive reciprocal lattice vectors and from them calculates the reciprocal lattice vectors $\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$.

On this page, the direction of the incoming electrons is given in terms of the primitive lattice vectors in reciprocal space, $H\vec{b}_1 + K\vec{b}_2 + L\vec{b}_3$. Usually the direction of the incoming electrons are given in terms of the conventional lattice vectors. Be aware that the [100] is a (usually) different direction if primitive lattice vectors are used than if conventional lattice vectors are used.

H: 1 K: 0 L: 0



[010] →

Primitive lattice vectors:

$\vec{a}_1$ =	4.12E-10	$\hat{x}$ +	0	$\hat{y}$ +	0	$\hat{z}$	[m]
$\vec{a}_2$ =	0	$\hat{x}$ +	4.12E-10	$\hat{y}$ +	0	$\hat{z}$	[m]
$\vec{a}_3$ =	0	$\hat{x}$ +	0	$\hat{y}$ +	4.12E-10	$\hat{z}$	[m]

Basis:

The positions of the atoms are given in fractional coodinates between -1 and 1.

Cs	0	$\vec{a}_1$ +	0	$\vec{a}_2$ +	0	$\vec{a}_3$
Cl	0.5	$\vec{a}_1$ +	0.5	$\vec{a}_2$ +	0.5	$\vec{a}_3$
		$\vec{a}_1$ +		$\vec{a}_2$ +		$\vec{a}_3$
		$\vec{a}_1$ +		$\vec{a}_2$ +		$\vec{a}_3$
		$\vec{a}_1$ +		$\vec{a}_2$ +		$\vec{a}_3$

submit

Neutron diffraction

Typically a nuclear reactor is used as the neutron source

There are different atomic form factors for neutrons than for x-rays.

Determine the positions of H in biological samples.

Can for example distinguish between Fe and Co which have similar atomic form factors for x-rays.

Structure factor for neutrons

The structure factor for neutrons can be calculated with the following formula,

$$F_{\vec{G}} = \sum_j b_j e^{-i\vec{G}\cdot\vec{r}_j} = \sum_j b_j \left(\cos\left(\vec{G}\cdot\vec{r}_j\right) - i\sin\left(\vec{G}\cdot\vec{r}_j\right)\right).$$

where $\vec{r}_j$ defines the position of the atom j and $\vec{G}$ is the reciprocal lattice vector. $\vec{b}_j$ is called the neutron scattering length, it depends on the spin-state of the neutron-nucleus system and the isotope the neutron is scattered from. The scattering lengths can be looked up at the NIST Center for Neutron Research.

The form below calculates the neutron structure factors. The script first calculates the reciprocal lattice vectors and from them calculates the reciprocal lattice vectors $\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$. The structure factors are calculated for a few reciprocal lattice vectors and listed in a table.

Primitive lattice vectors:

$\vec{a}_1 =$	4.12E-10	$\hat{x}+$	0	$\hat{y}+$	0	$\hat{z}$	[m]
$\vec{a}_2 =$	0	$\hat{x}+$	4.12E-10	$\hat{y}+$	0	$\hat{z}$	[m]
$\vec{a}_3 =$	0	$\hat{x}+$	0	$\hat{y}+$	4.12E-10	$\hat{z}$	[m]

Basis:

The positions of the atoms are given in fractional coodinates between -1 and 1.

Pb	0	$\vec{a}_1+$	0	$\vec{a}_2+$	0	$\vec{a}_3$
Ti	0.5	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0.5	$\vec{a}_1+$	0	$\vec{a}_2+$	0.5	$\vec{a}_3$
O	0.5	$\vec{a}_1+$	0.5	$\vec{a}_2+$	0	$\vec{a}_3$
		$\vec{a}_1+$		$\vec{a}_2+$		$\vec{a}_3$
		$\vec{a}_1+$		$\vec{a}_2+$		$\vec{a}_3$
		$\vec{a}_1+$		$\vec{a}_2+$		$\vec{a}_3$

submit

Atomic beams

Hydrogen and Helium are used for diffraction studies

$$E = \tfrac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2}$$

Low energies can be used for delicate samples.
Measure the surface like LEED.

Forbidden reflections

Primitive lattice vectors:

$\vec{a}_1 =$ 4.12E-10 $\hat{x} +$ 0 $\hat{y}$ [m]
$\vec{a}_2 =$ 0 $\hat{x} +$ 6.12E-10 $\hat{y}$ [m]

Basis:
The positions of the atoms are given in fractional coodinates between -1 and 1.

C	0	$\vec{a}_1 +$	0	$\vec{a}_2$	
C	0.5	$\vec{a}_1 +$	0.5	$\vec{a}_2$	
	0.2	$\vec{a}_1 +$	0.3	$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	
		$\vec{a}_1 +$		$\vec{a}_2$	

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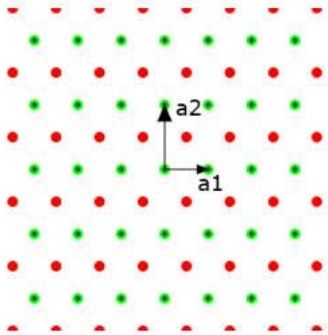
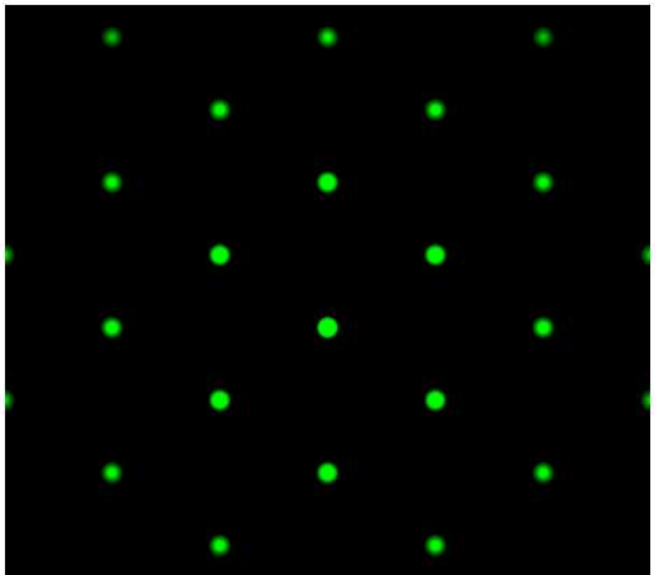


Primitive reciprocal lattice vectors

$\vec{b}_1 = 2\pi \frac{R\,\vec{a}_2}{\vec{a}_1 \cdot R\,\vec{a}_2} =$1.525e+10 $\hat{k}_x +$ 0.000 $\hat{k}_y$ [m^{-1}]
$\vec{b}_2 = 2\pi \frac{R\,\vec{a}_1}{\vec{a}_1 \cdot R\,\vec{a}_2} =$ 0.000 $\hat{k}_x +$ -1.027e+10 $\hat{k}_y$ [m^{-1}]
with $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

Low Energy
Electron Diffraction



Forbidden reflections

$$n_{u.c.}(\vec{r}) = \sum_j Z_j \delta(\vec{r} - \vec{r}_j)$$

Primitive reciprocal lattice vectors

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 3.939\ \hat{k}_x + -2.275\text{e+}10\ \hat{k}_y + 0.000\ \hat{k}_z\ [\text{m}^{-1}]$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 3.939\ \hat{k}_x + 2.275\ \hat{k}_y + 0.000\ \hat{k}_z\ [\text{m}^{-1}]$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0.000\ \hat{k}_x + 0.000\ \hat{k}_y + 1.212\text{e+}10\ \hat{k}_z\ [\text{m}^{-1}]$$

$$n_{\vec{G}} = \sum_j Z_j \exp(-i\vec{G} \cdot \vec{r}_j)$$

Structure factors

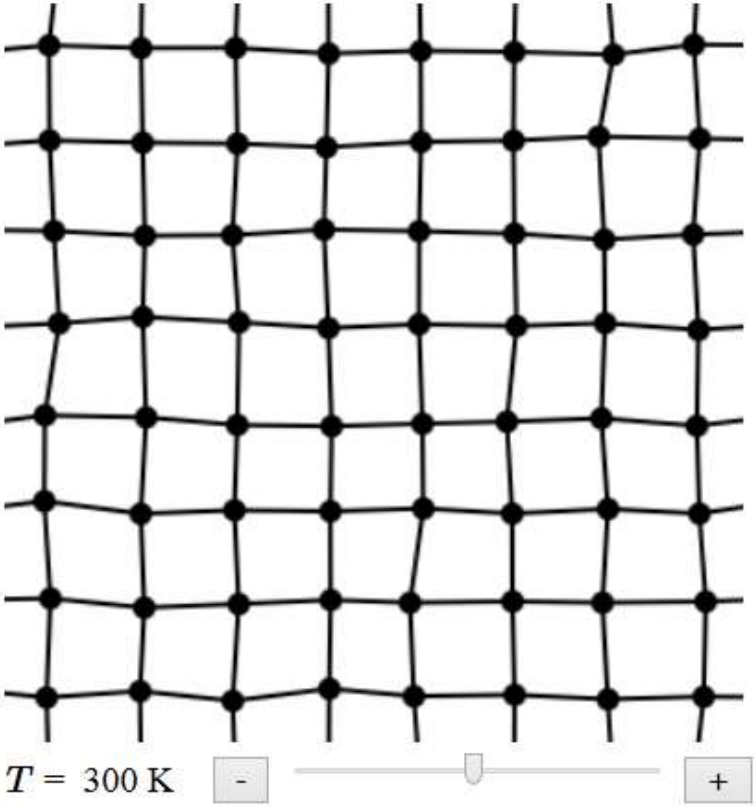
The value of $|n_{\vec{G}}|$ for the 000 diffraction peak is the total number of electrons in the primitive unit cell. The intensities of the peaks in an x-ray diffraction experiment are proportional to $|n_{\vec{G}}|^2$. Note that elements with more electrons produce stronger diffraction intensities.

hkl	$\|\vec{G}\|$ Å^{-1}	$\|n_{\vec{G}}\|$	$\|n_{\vec{G}}\|^2$	Re$\{n_{\vec{G}}\}$	Im$\{n_{\vec{G}}\}$
000	0.000	75.94	5767	75.94	0.000
0-10	4.549e-10	37.87	1434	-37.87	0.02201
010	4.549e-10	37.87	1434	-37.87	-0.02201
0-20	9.098e-10	38.17	1457	-38.17	0.04379
020	9.098e-10	38.17	1457	-38.17	-0.04379
0-30	1.365e-9	75.94	5767	75.94	-0.1318
030	1.365e-9	75.94	5767	75.94	0.1318
0-3-1	1.212	0.3909	0.1528	0.02780	0.3899
0-31	1.212	0.3914	0.1532	-0.02727	0.3904
0-2-1	1.212	42.85	1836	-7.648	42.16
0-21	1.212	42.74	1827	7.551	42.07
0-1-1	1.212	43.01	1850	7.610	-42.33
0-11	1.212	42.96	1845	-7.561	-42.29
00-1	1.212	8.896e-8	7.914e-15	-1.573e-8	8.756e-8
001	1.212	8.896e-8	7.914e-15	-1.573e-8	-8.756e-8
01-1	1.212	42.96	1845	-7.561	42.29
011	1.212	43.01	1850	7.610	42.33
02-1	1.212	42.74	1827	7.551	-42.07
021	1.212	42.85	1836	-7.648	-42.16
03-1	1.212	0.3914	0.1532	-0.02727	-0.3904

Phonons

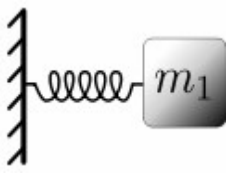
Normal Modes and Phonons

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



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

Vibrations of a mass on a spring



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

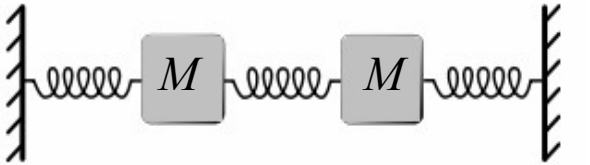
The solution has the form

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

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

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

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

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

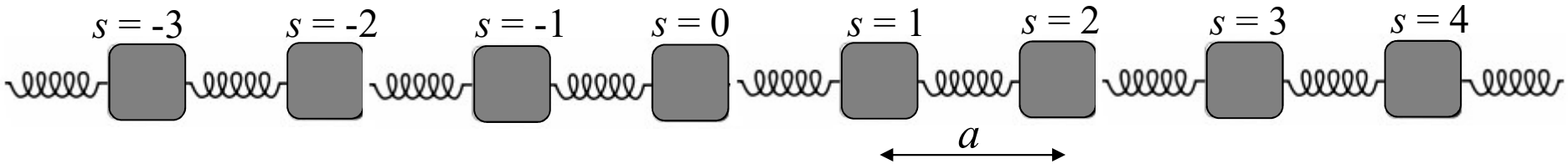
$$-\omega^2 MA_1e^{i\omega t} = -2CA_1e^{i\omega t} + CA_2e^{i\omega t}$$
$$-\omega^2 MA_2e^{i\omega t} = -2CA_2e^{i\omega t} + CA_1e^{i\omega t}$$

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

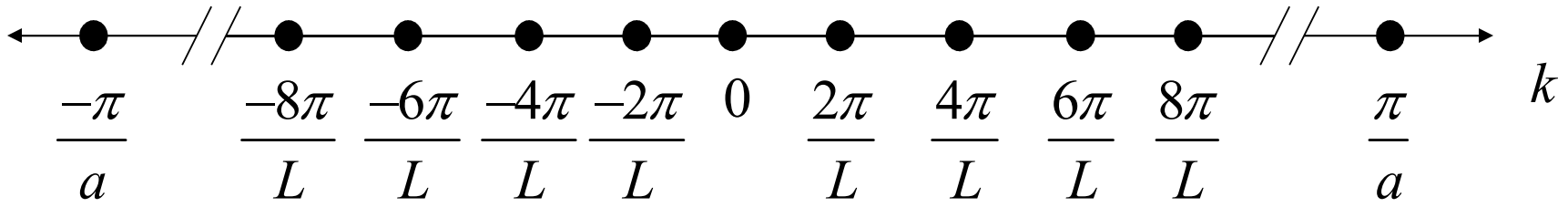
Find the eigenvectors of this matrix

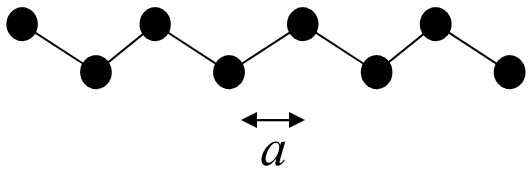
The masses oscillate with the same frequency but different phases

Linear Chain

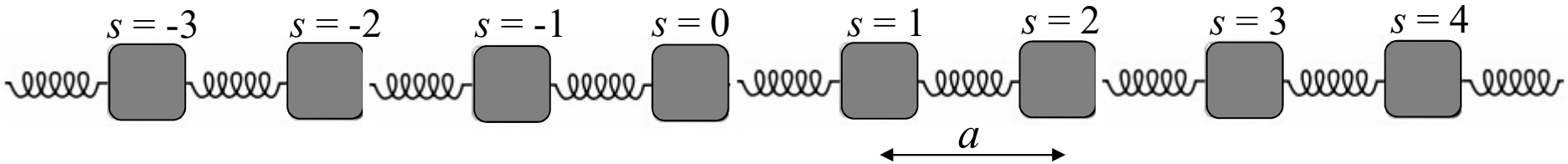


solution: $u_s = A_k e^{i(ksa-\omega t)} = A_k e^{iksa} e^{-i\omega t}$





Linear Chain



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

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

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

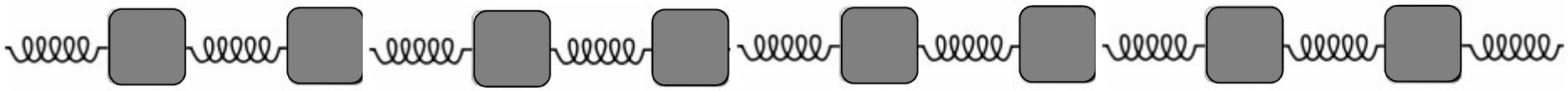
$$-\omega^2 m = C(e^{ika} - 2 + e^{-ika})$$

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

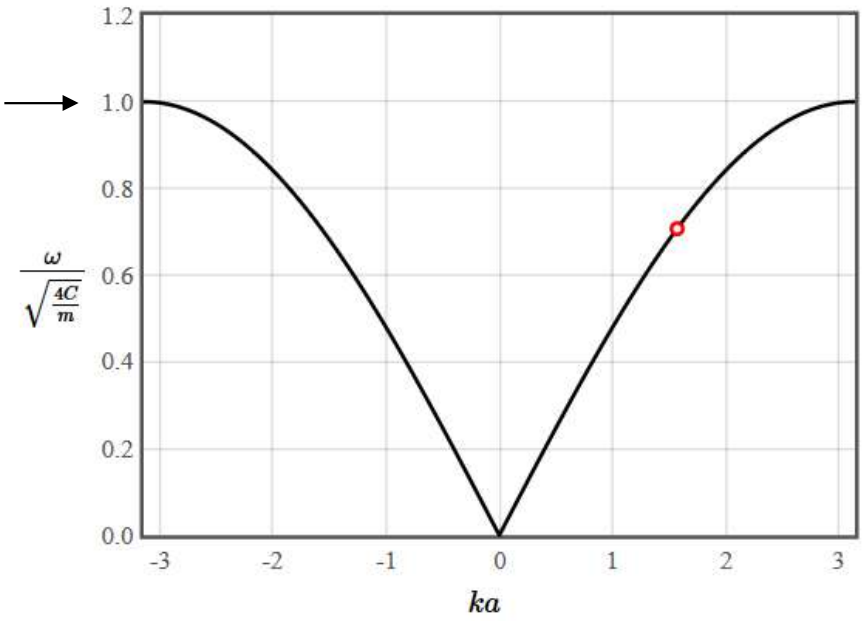
$$\sin^2\frac{ka}{2} = \frac{1}{2}(1-\cos ka)$$

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

Linear Chain - dispersion relation



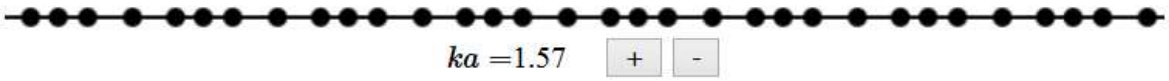
Max. freq. →



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

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

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

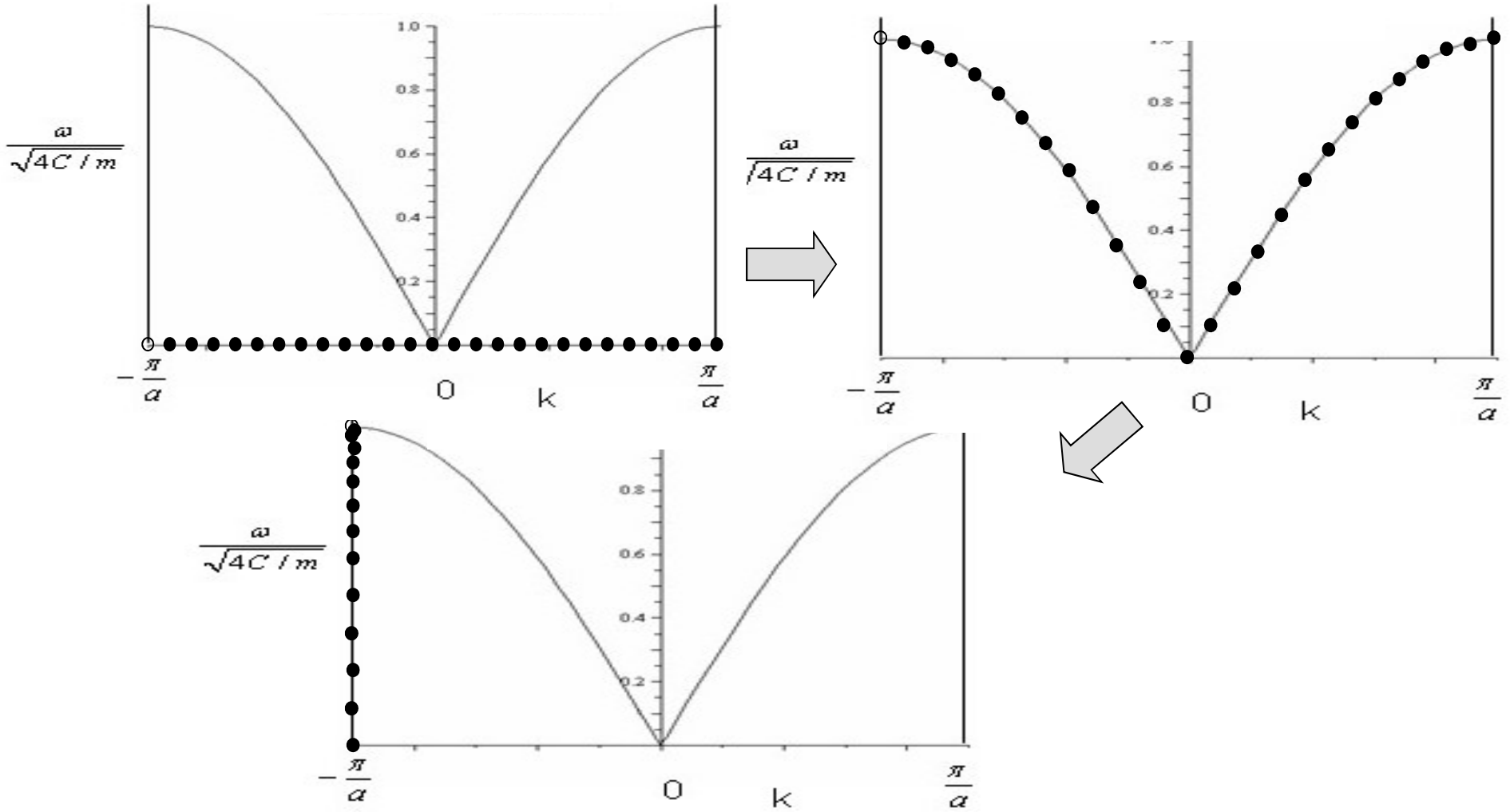


speed of sound = $\sqrt{\frac{C}{m}}a$

Linear Chain - density of states

Determine the density of states numerically

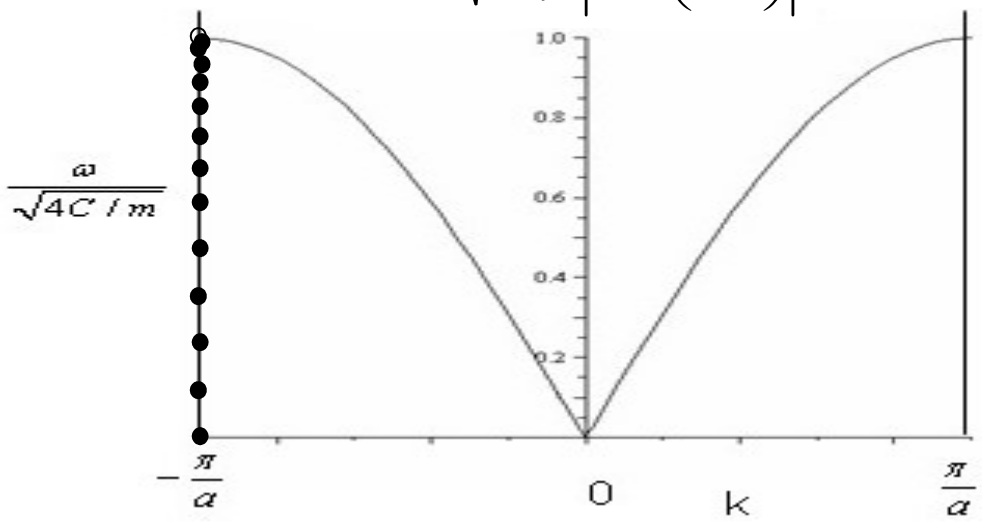
$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



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

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

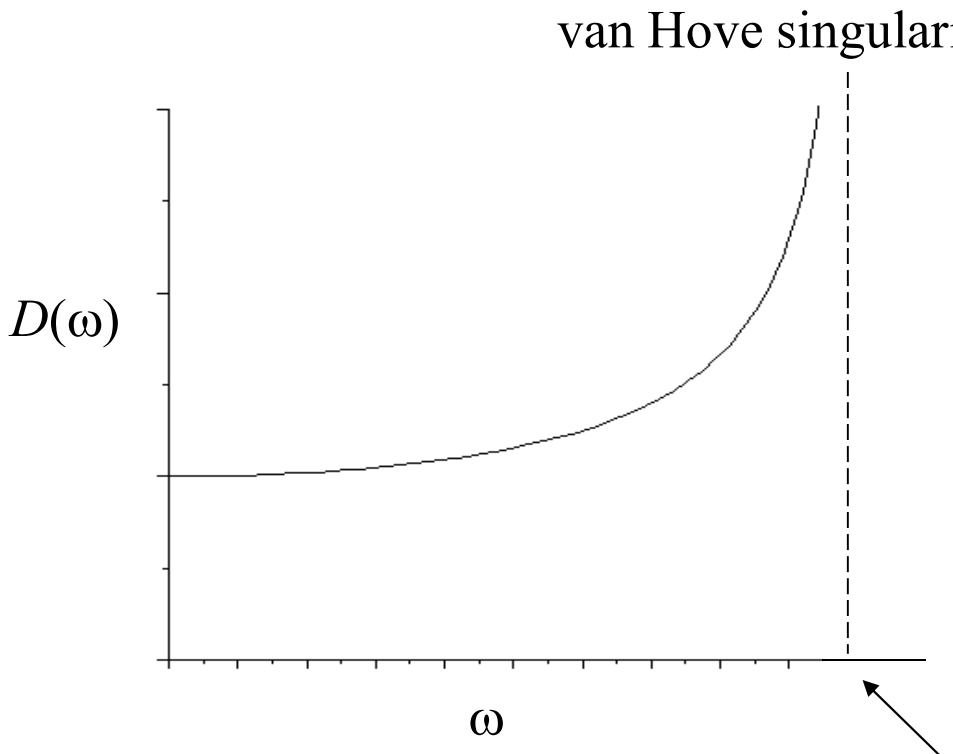
$$D(k) = \frac{1}{\pi}$$

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

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

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

density of states



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

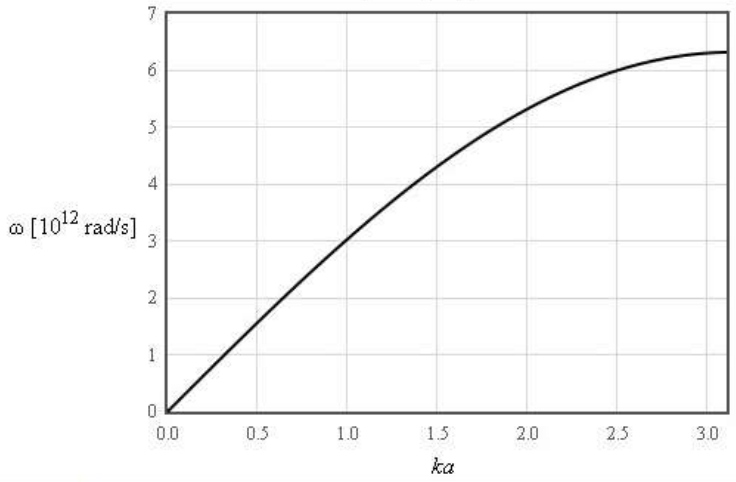
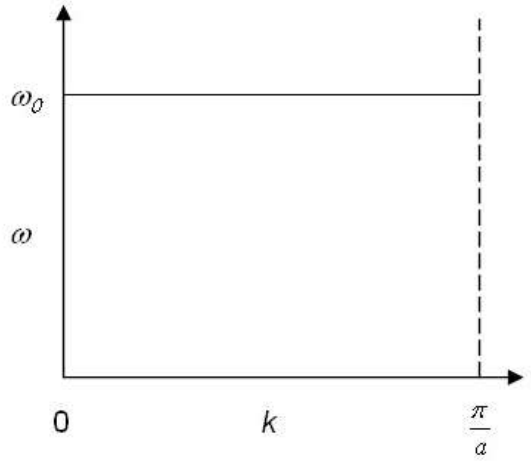
$$D(k) = \frac{1}{\pi}$$

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

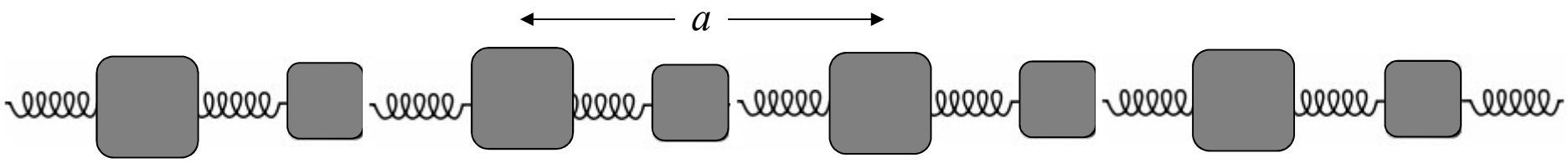
$$d\omega = a\sqrt{\frac{C}{m}}\cos\left(\frac{ka}{2}\right)dk$$

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

Phonons

	Linear Chain	**Einstein Model**	
	$m\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$	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	$\omega = \sqrt{\frac{4C}{m}}\left\lvert\sin\left(\frac{ka}{2}\right)\right\rvert$ 		ω_D ω

Linear chain M_1 and M_2



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

$2N$ modes

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

assume harmonic solutions

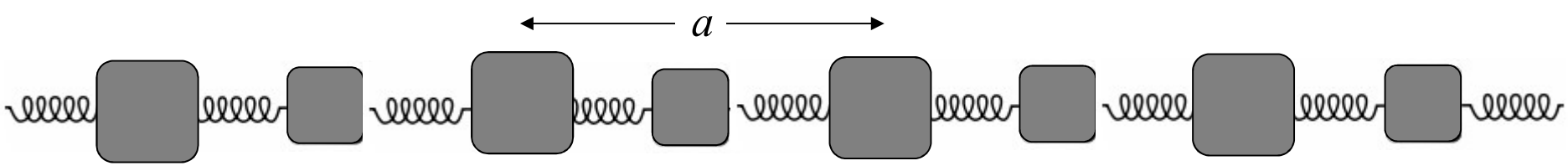
$$u_s = u_k e^{i(ksa - \omega t)}$$

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

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

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

Linear chain M_1 and M_2



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

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

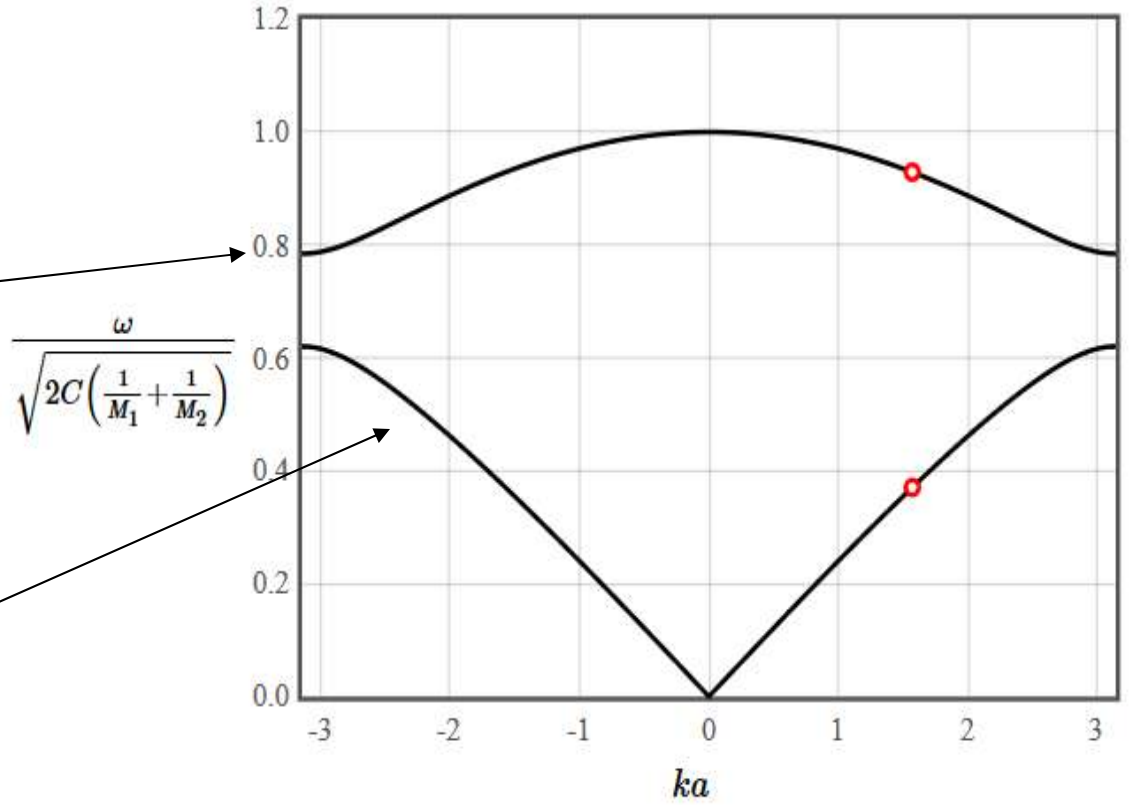
$$M_1 M_2 \omega^4 - 2C\left(M_1 + M_2\right)\omega^2 + 2C^2\left(1-\cos(ka)\right) = 0$$

dispersion relation

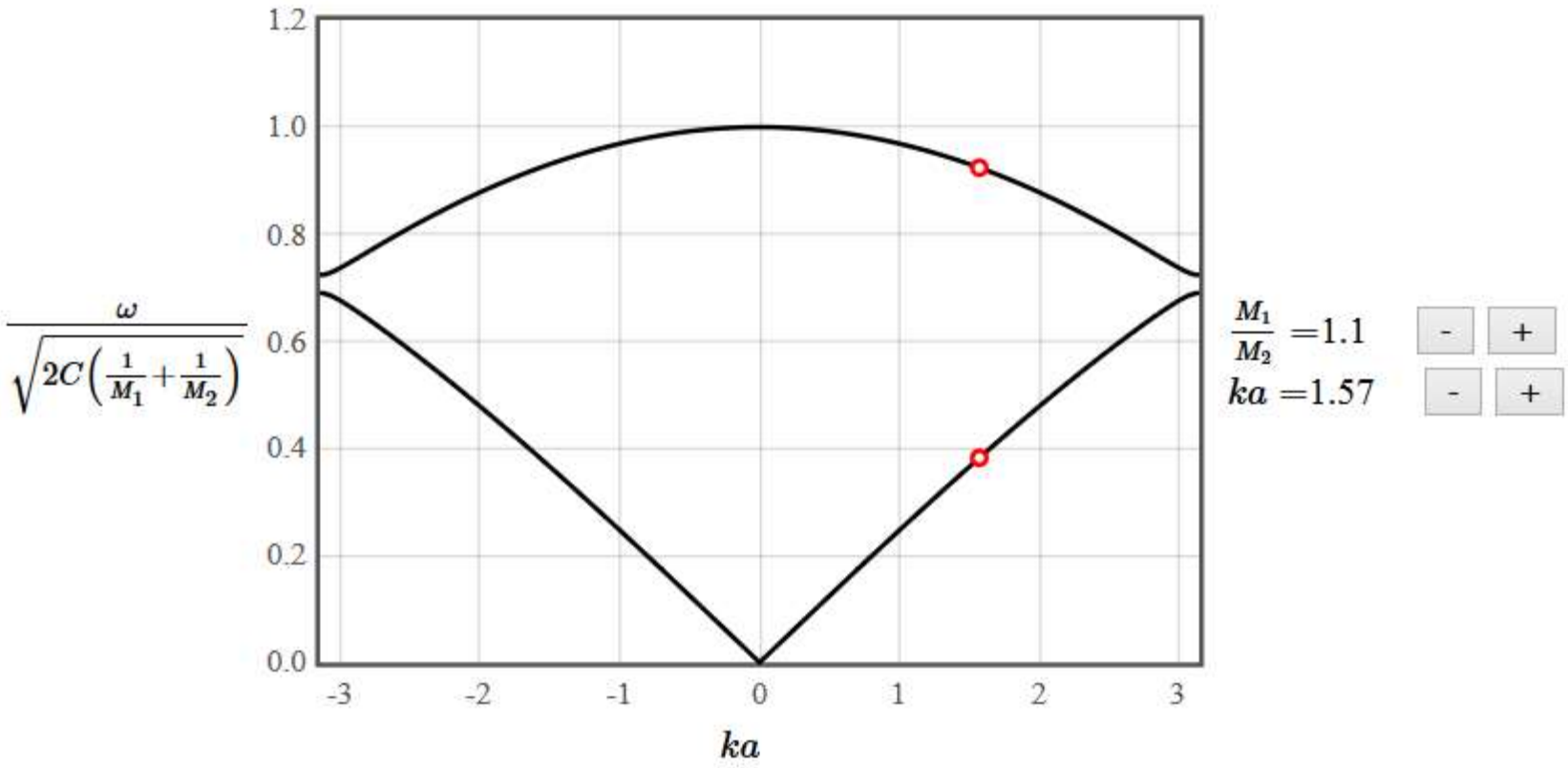
$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2\left(\frac{ka}{2}\right)}{M_1 M_2}}$$

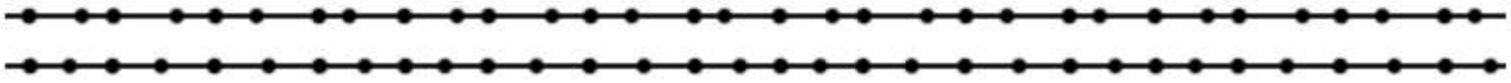
Optical phonon branch

Acoustic phonon branch



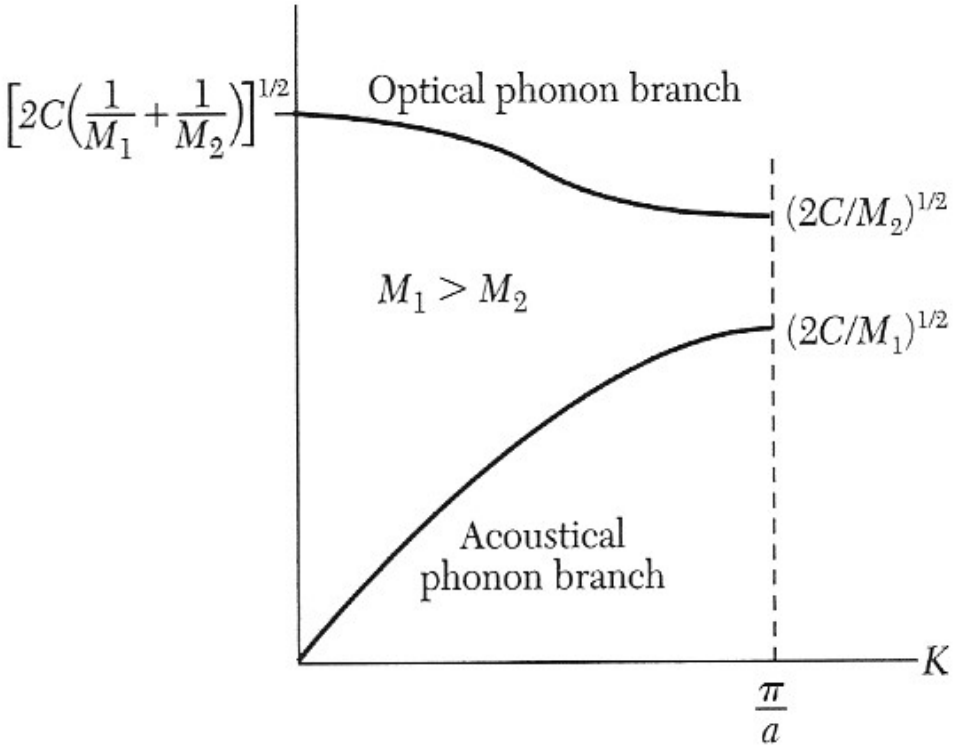
normal modes

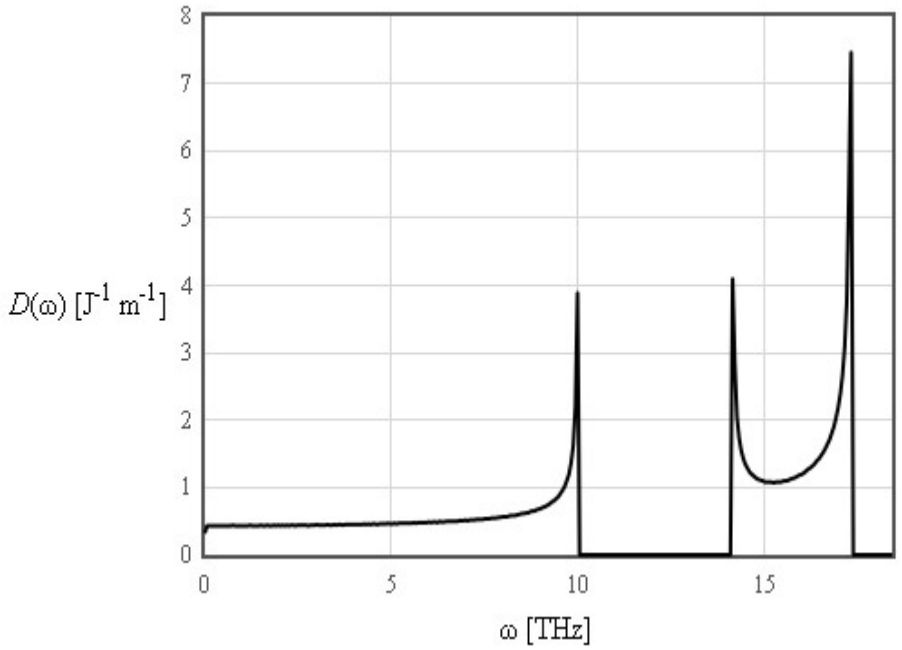




http://lampx.tugraz.at/~hadley/ss1/phonons/1d/1d2m.php

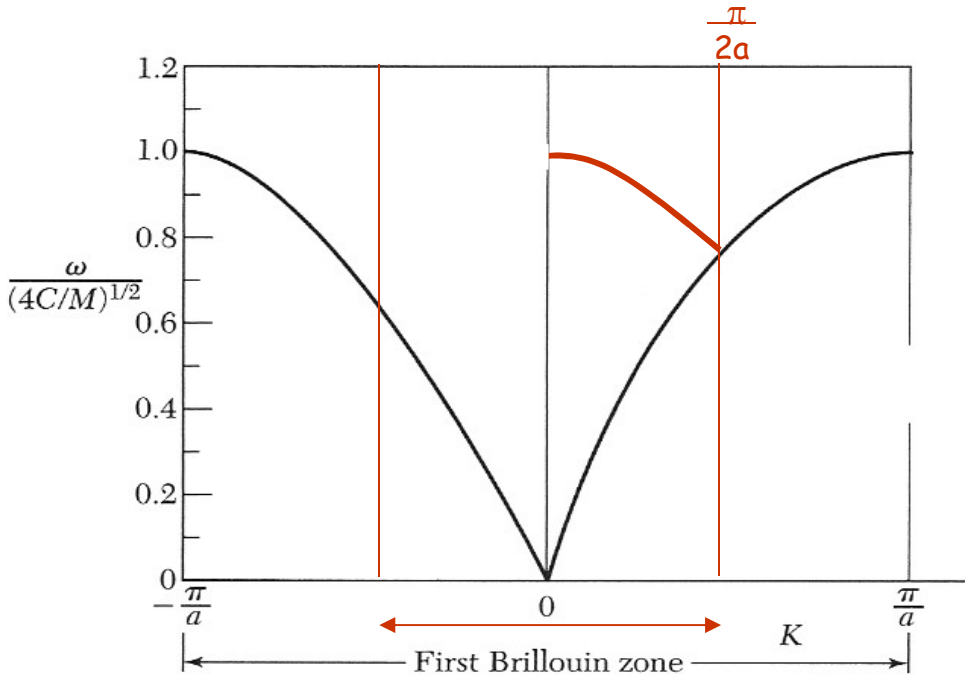
density of states



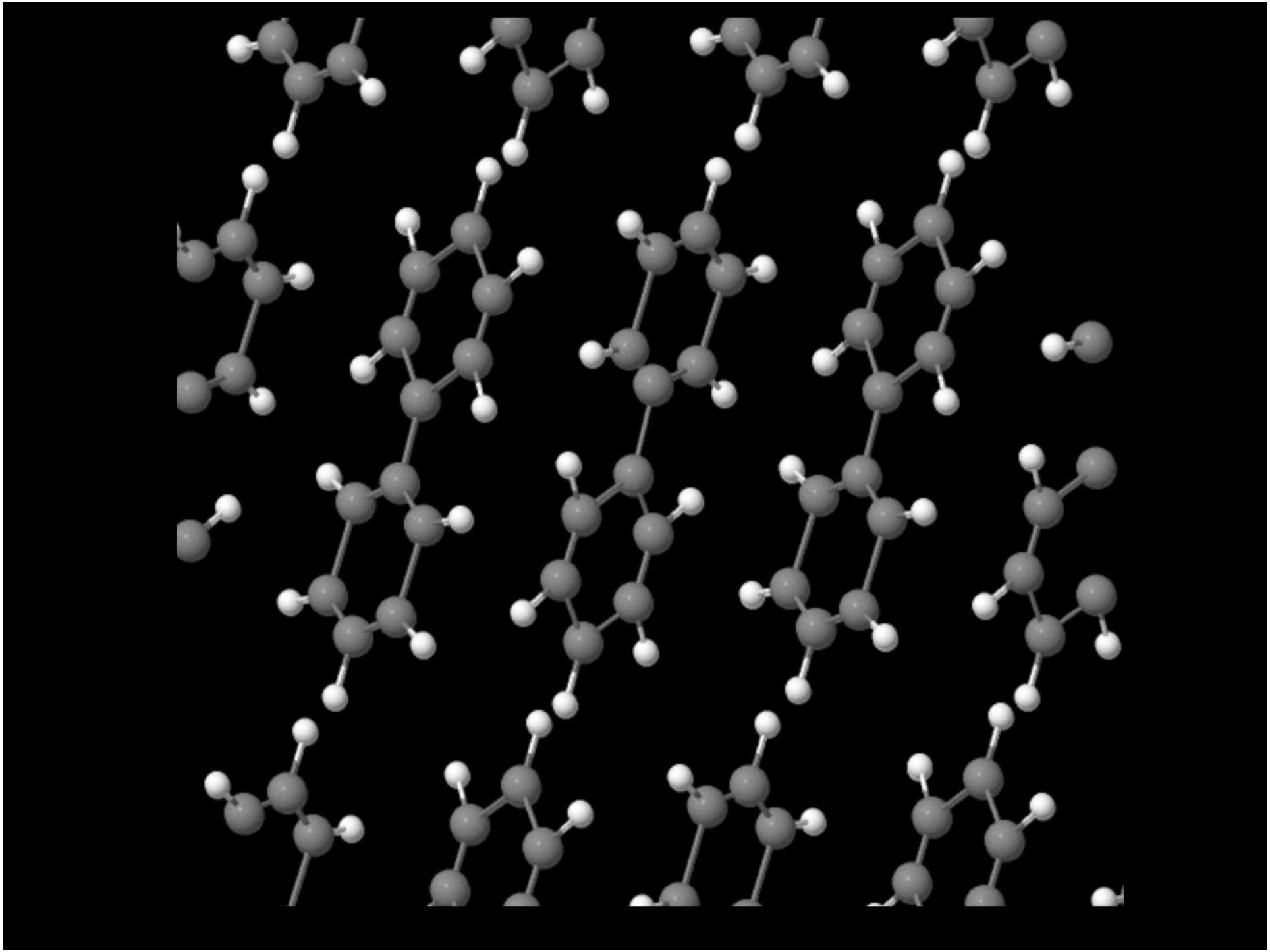


$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2 ka}{M_1 M_2}}$$

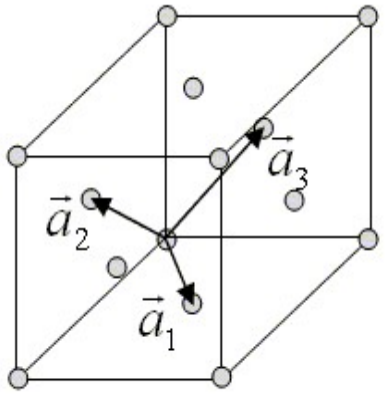
Linear chain M_1 and M_2



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

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

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

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

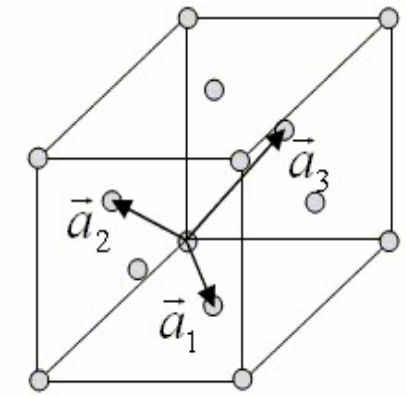
These are eigenfunctions of T.

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

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

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

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.

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

$$\begin{vmatrix} 4-\cos\left(\frac{k_x a}{2}+\frac{k_y a}{2}\right)-\cos\left(\frac{k_x a}{2}+\frac{k_z a}{2}\right)-\cos\left(\frac{k_x a}{2}-\frac{k_y a}{2}\right)-\cos\left(\frac{k_x a}{2}-\frac{k_z a}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_x a}{2}+\frac{k_y a}{2}\right)+\cos\left(\frac{k_x a}{2}-\frac{k_y a}{2}\right) & -\cos\left(\frac{k_x a}{2}+\frac{k_z a}{2}\right)+\cos\left(\frac{k_x a}{2}-\frac{k_z a}{2}\right) \\ -\cos\left(\frac{k_x a}{2}+\frac{k_y a}{2}\right)+\cos\left(\frac{k_x a}{2}-\frac{k_y a}{2}\right) & 4-\cos\left(\frac{k_y a}{2}+\frac{k_z a}{2}\right)-\cos\left(\frac{k_y a}{2}+\frac{k_x a}{2}\right)-\cos\left(\frac{k_y a}{2}-\frac{k_x a}{2}\right)-\cos\left(\frac{k_y a}{2}-\frac{k_z a}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_y a}{2}+\frac{k_z a}{2}\right)+\cos\left(\frac{k_y a}{2}-\frac{k_z a}{2}\right) \\ -\cos\left(\frac{k_x a}{2}+\frac{k_z a}{2}\right)+\cos\left(\frac{k_x a}{2}-\frac{k_z a}{2}\right) & -\cos\left(\frac{k_y a}{2}+\frac{k_z a}{2}\right)+\cos\left(\frac{k_y a}{2}-\frac{k_z a}{2}\right) & 4-\cos\left(\frac{k_z a}{2}+\frac{k_x a}{2}\right)-\cos\left(\frac{k_z a}{2}+\frac{k_y a}{2}\right)-\cos\left(\frac{k_z a}{2}-\frac{k_y a}{2}\right)-\cos\left(\frac{k_z a}{2}-\frac{k_y a}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} \end{vmatrix} = 0$$

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

For every k there are 3 solutions for ω.