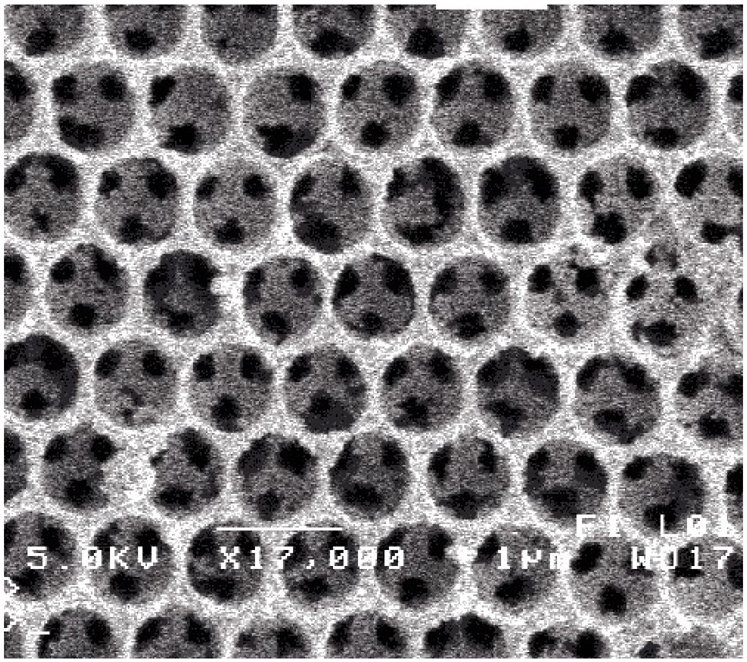
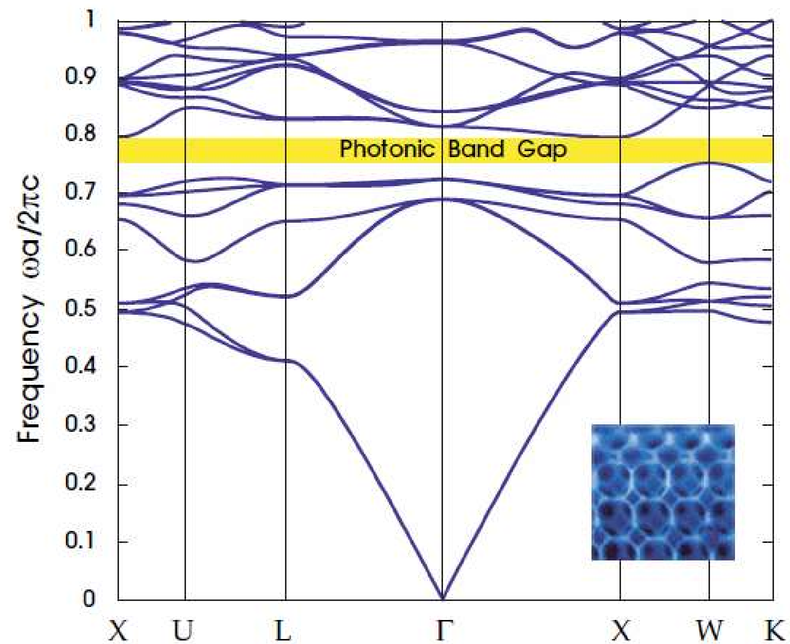
Photons

Inverse opal photonic crystal





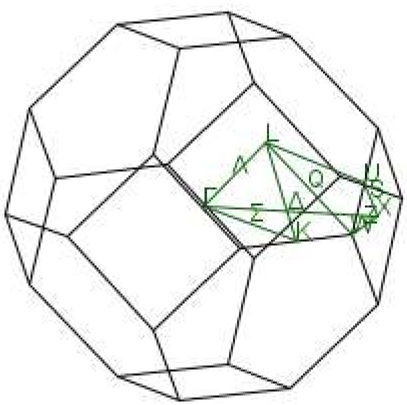
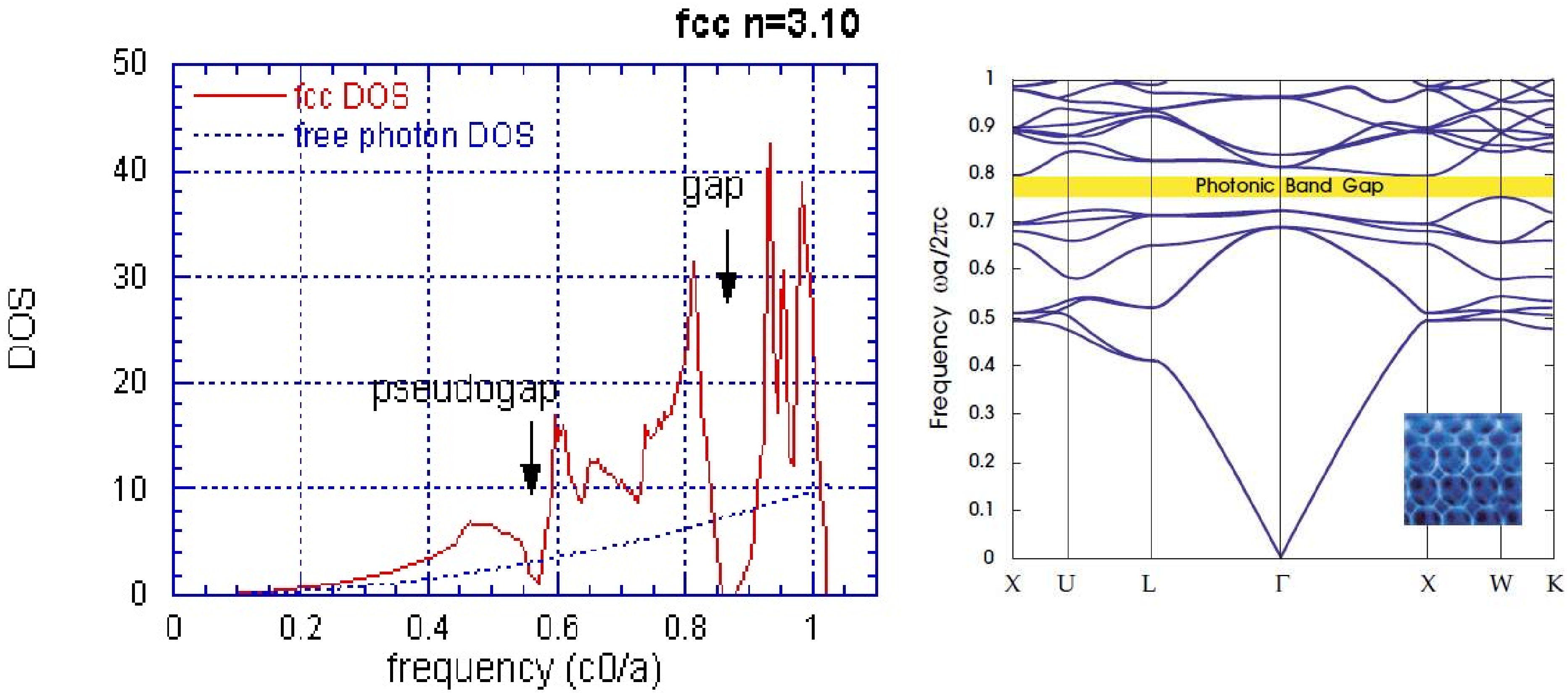


Figure 8: The photonic band structure for the lowest bands of an "inverse opal" structure: a face-centered cubic (fcc) lattice of close-packed air spheres in dielectric ($\varepsilon = 13$). (Inset shows fabricated structure from figure 9.) There is a complete photonic band gap (yellow) between the eighth and ninth bands. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points; see appendix B for a discussion of the Brillouin zone of an fcc lattice.

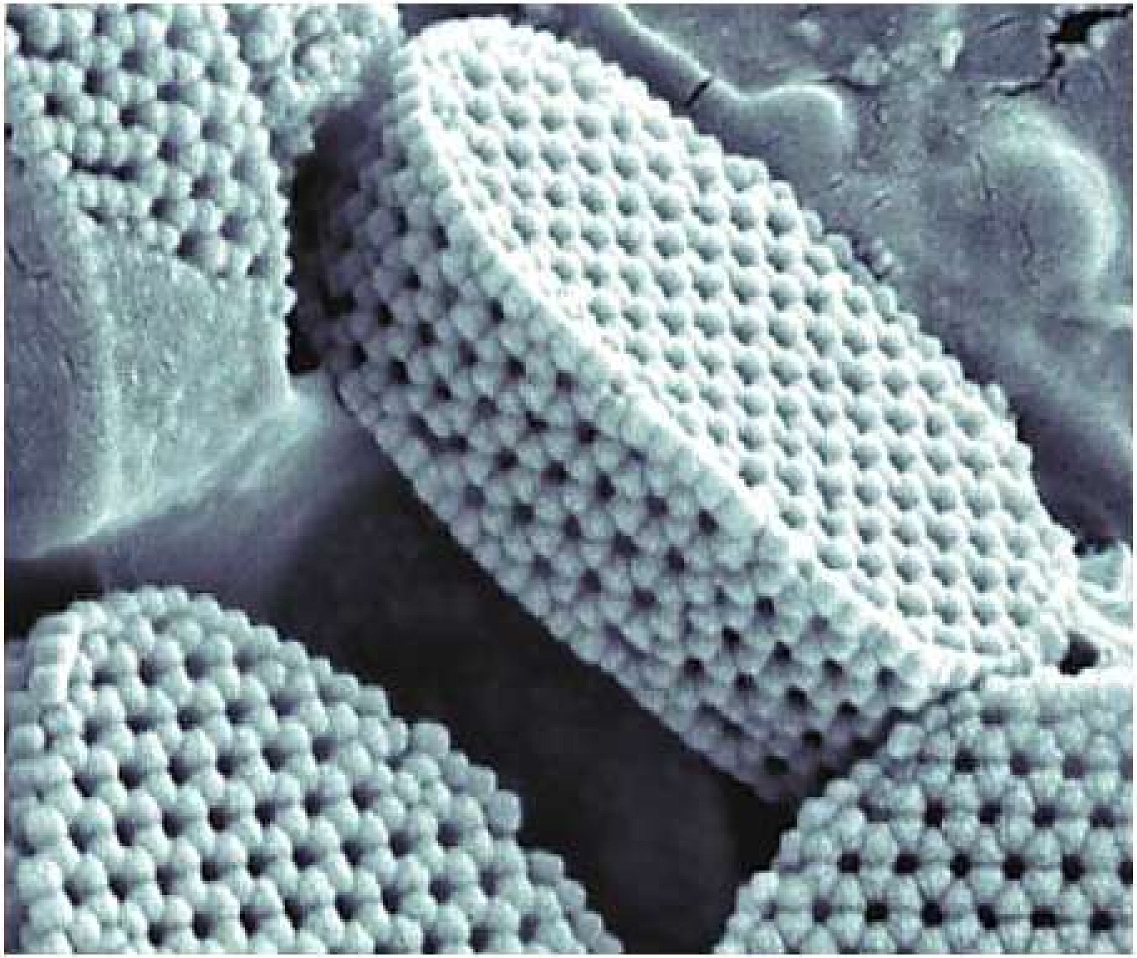
http://ab-initio.mit.edu/book

Photon density of states

Diffraction causes gaps in the density of modes for *k* vectors near the planes in reciprocal space where diffraction occurs.



photon density of states for voids in an fcc lattice
http://www.public.iastate.edu/~cmpexp/groups/PBG/pres_mit_short/sld002.htm

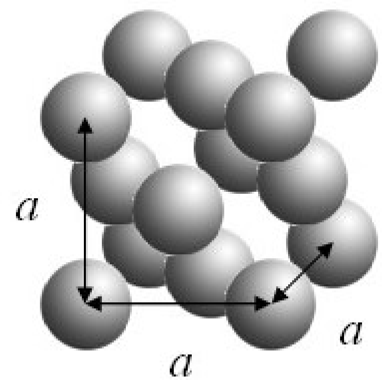


The alga Calyptrolithophora papillifera is encased in a shell of calcite crystals with a two-layer structure (visible on oblique face). Calculations show that this protective covering reflects ultraviolet light. Image Credit: J. Young/Natural History Museum, London

http://www.physicscentral.com/explore/pictures/algae.cfm

Spheres on any 3-D Bravais lattice

$$c(\vec{r})^2 \nabla^2 A_j = \frac{d^2 A_j}{dt^2}$$



$$c(\vec{r})^2 = \sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = c_1^2 + \frac{4\pi\left(c_2^2 - c_1^2\right)}{V} \sum_{\vec{G}} \frac{\sin\left(|G|R\right) - |G|R\cos\left(|G|R\right)}{|G|^3} \exp\left(i\vec{G}\cdot\vec{r}\right)$$

Plane wave method

$$c(\vec{r})^2 \nabla^2 A_j = \frac{d^2 A_j}{dt^2}$$

$$c(\vec{r})^2 = \sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \qquad A_j = \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

$$\sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \sum_{\vec{\kappa}} \left(-\kappa^2\right) A_{\vec{\kappa}} e^{i\left(\vec{\kappa}\cdot\vec{r}-\omega t\right)} = -\omega^2 \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

$$\sum_{\vec{\kappa}} \sum_{\vec{G}} \left(-\kappa^2\right) b_{\vec{G}} A_{\vec{\kappa}} e^{i\left(\vec{G}\cdot\vec{r}+\vec{\kappa}\cdot\vec{r}-\omega t\right)} = -\omega^2 \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

collect like terms: $\vec{G}+\vec{\kappa}=\vec{k} \quad \Rightarrow \quad \vec{\kappa}=\vec{k}-\vec{G}$

Central equations: $$\sum_{\vec{G}} \left(\vec{k}-\vec{G}\right)^2 b_{\vec{G}} A_{\vec{k}-\vec{G}} = \omega^2 A_{\vec{k}}$$

Plane wave method

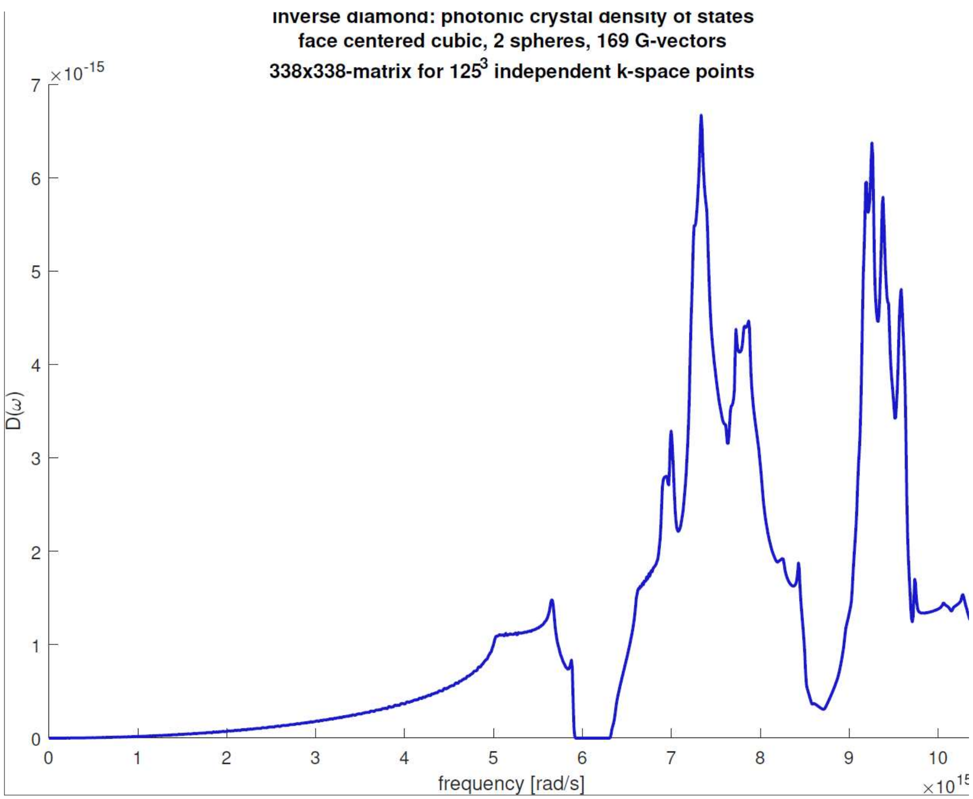
Central equations: $$\sum_{\vec{G}} \left(\vec{k}-\vec{G}\right)^2 b_{\vec{G}} A_{\vec{k}-\vec{G}} = \omega^2 A_{\vec{k}}$$

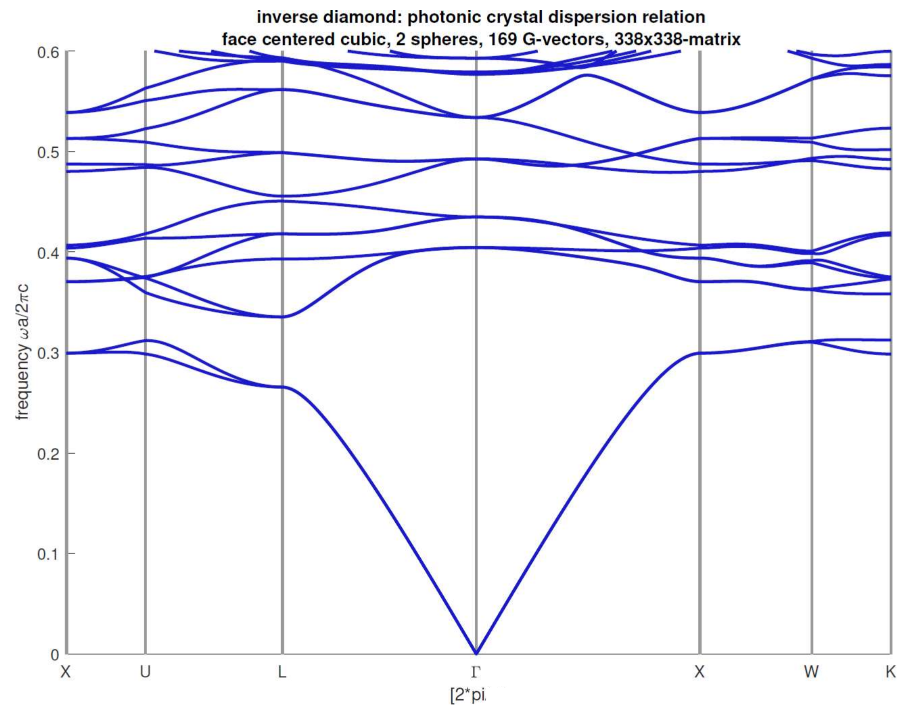
Choose a *k* value inside the 1st Brillouin zone. The coefficient A_k is coupled by the central equations to coefficients A_k outside the 1st Brillouin zone. Write these coupled equations in matrix form.

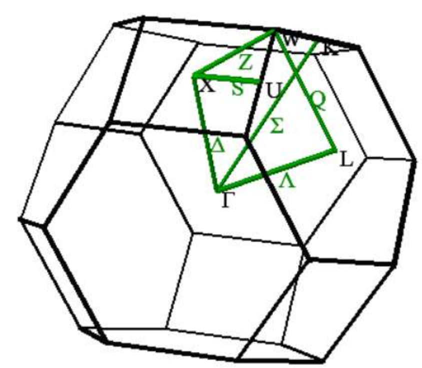
$$\begin{bmatrix}
\left(\vec{k}+\vec{G}_2\right)^2 b_0-\omega^2 & \left(\vec{k}+\vec{G}_2-\vec{G}_1\right)^2 b_{\vec{G}_1} & k^2 b_{\vec{G}_2} & \left(\vec{k}+\vec{G}_2-\vec{G}_3\right)^2 b_{\vec{G}_3} & \left(\vec{k}+\vec{G}_2-\vec{G}_4\right)^2 b_{\vec{G}_4} \\
\left(\vec{k}+2\vec{G}_1\right)^2 b_{-\vec{G}_1} & \left(\vec{k}+\vec{G}_1\right)^2 b_0-\omega^2 & k^2 b_{\vec{G}_1} & \left(\vec{k}+\vec{G}_1-\vec{G}_2\right)^2 b_{\vec{G}_2} & \left(\vec{k}+\vec{G}_1-\vec{G}_3\right)^2 b_{\vec{G}_3} \\
\left(\vec{k}+\vec{G}_2\right)^2 b_{-\vec{G}_2} & \left(\vec{k}+\vec{G}_1\right)^2 b_{-\vec{G}_1} & k^2 b_0-\omega^2 & \left(\vec{k}-\vec{G}_1\right)^2 b_{\vec{G}_1} & \left(\vec{k}-\vec{G}_2\right)^2 b_{\vec{G}_2} \\
\left(\vec{k}-\vec{G}_1+\vec{G}_3\right)^2 b_{-\vec{G}_3} & \left(\vec{k}-\vec{G}_1+\vec{G}_2\right)^2 b_{-\vec{G}_2} & k^2 b_{-\vec{G}_1} & \left(\vec{k}-\vec{G}_1\right)^2 b_0-\omega^2 & \left(\vec{k}-2\vec{G}_1\right)^2 b_{\vec{G}_1} \\
\left(\vec{k}-\vec{G}_2+\vec{G}_4\right)^2 b_{-\vec{G}_4} & \left(\vec{k}-\vec{G}_2+\vec{G}_3\right)^2 b_{-\vec{G}_3} & k^2 b_{-\vec{G}_2} & \left(\vec{k}-\vec{G}_2+\vec{G}_1\right)^2 b_{-\vec{G}_1} & \left(\vec{k}-\vec{G}_2\right)^2 b_0-\omega^2
\end{bmatrix}
\begin{bmatrix} A_{k+G_2} \\ A_{k+G_1} \\ A_k \\ A_{k-G_1} \\ A_{k-G_2} \end{bmatrix} = 0$$

There is a matrix like this for every *k* value in the 1st Brillouin zone.

Inverse diamond

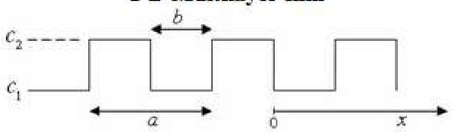






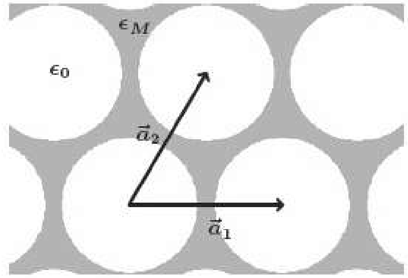
Solved by a student with the plane wave method

1-D Multilayer film

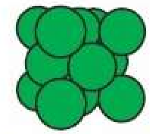


1-D Multilayer film

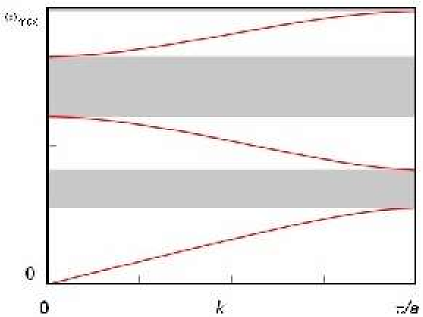
2-D triangular array of air holes



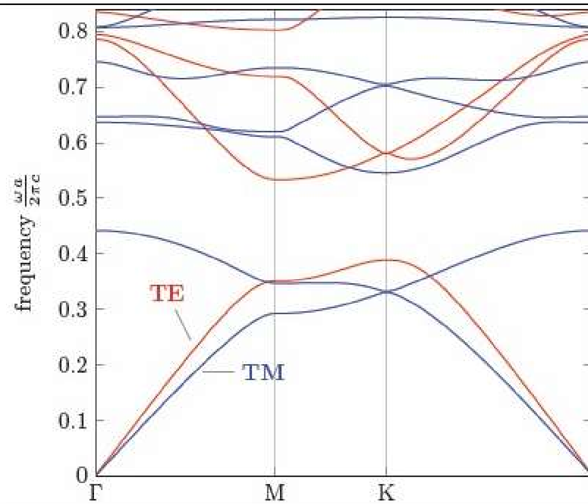
fcc

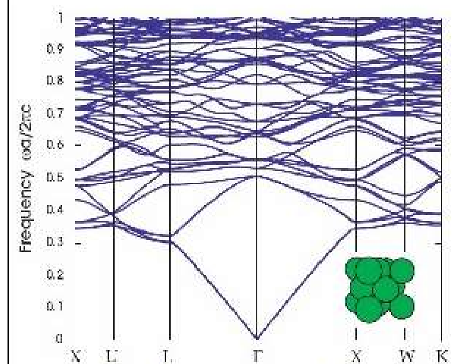


http://ab-initio.mit.edu/book



Calculate ω(k)





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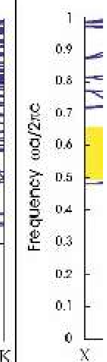
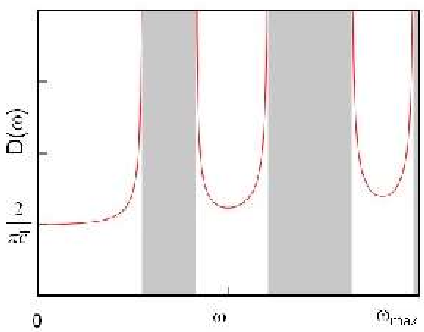
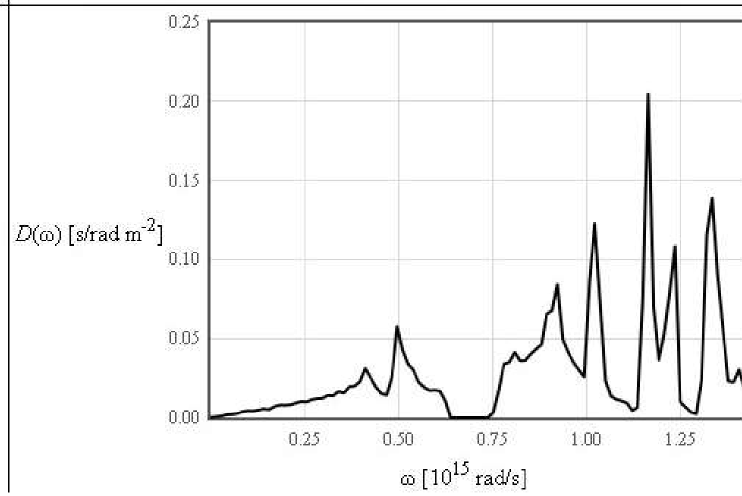
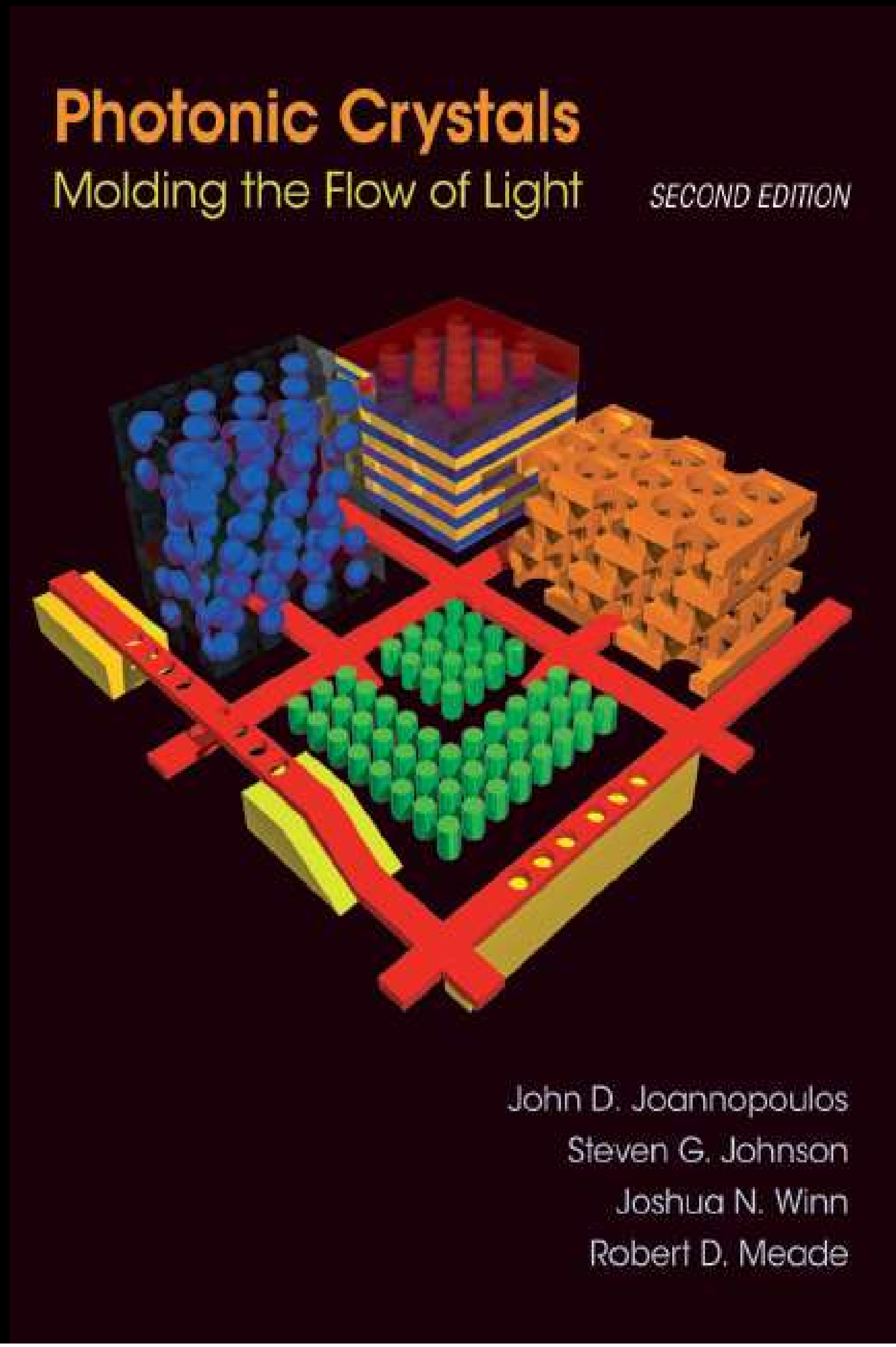




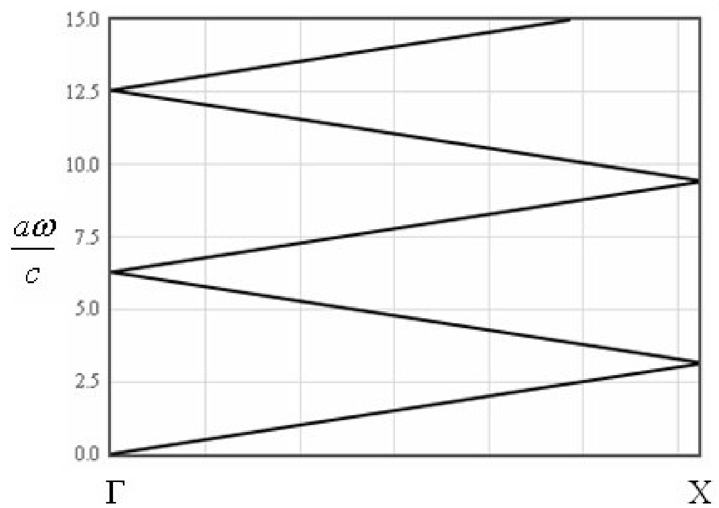
Calculate DoS

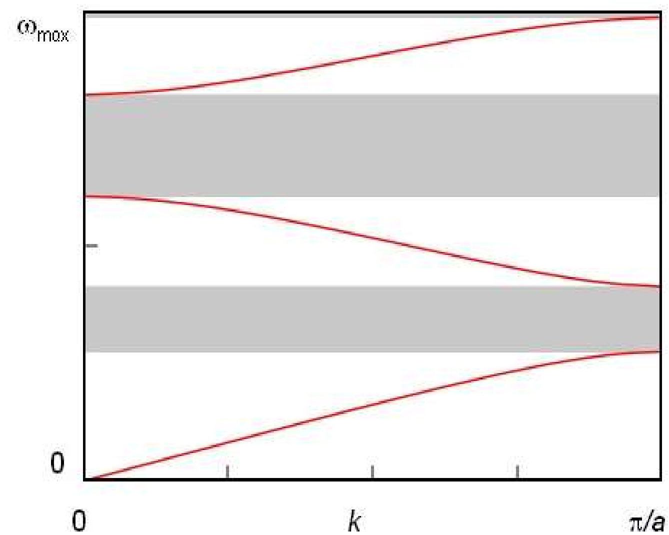


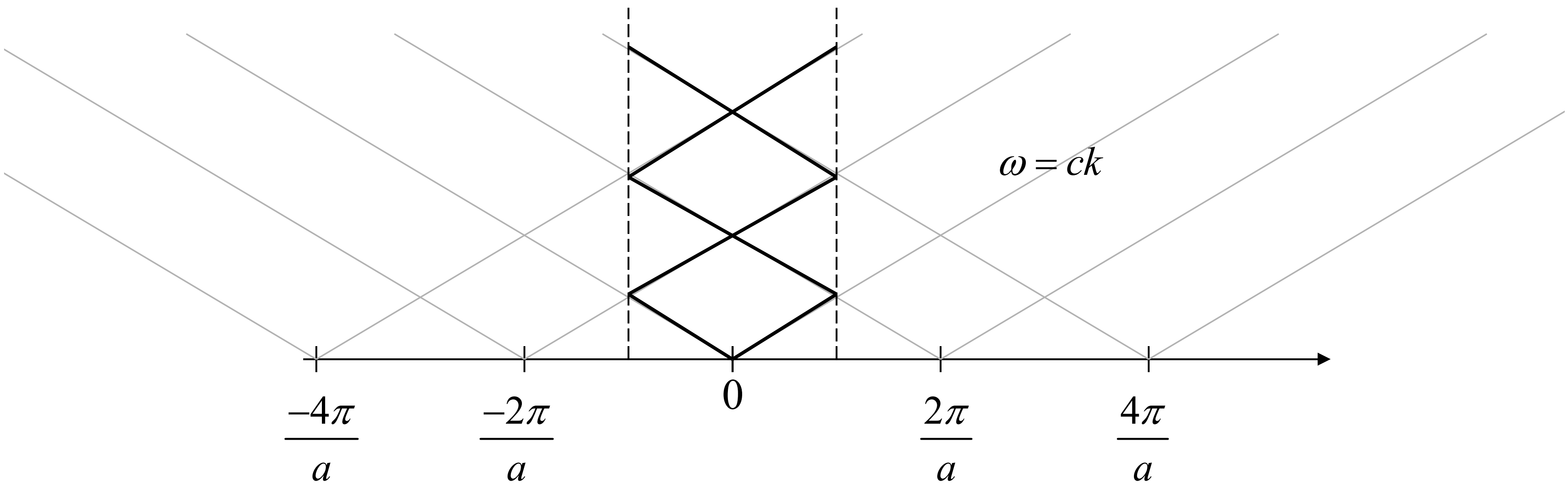
http://lampx.tugraz.at/~hadley/ss1/emfield/photonic_crystals/photonic_table.html http://ab-initio.mit.edu/book/



Empty lattice approximation

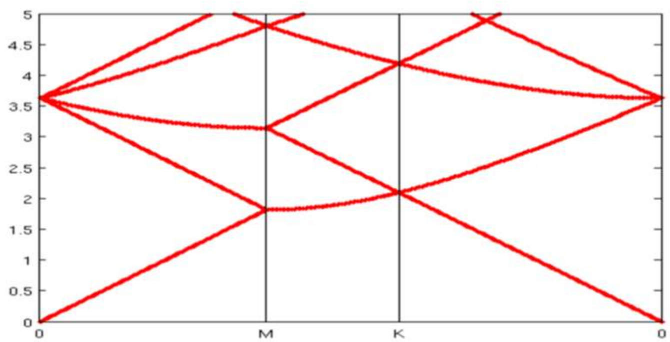


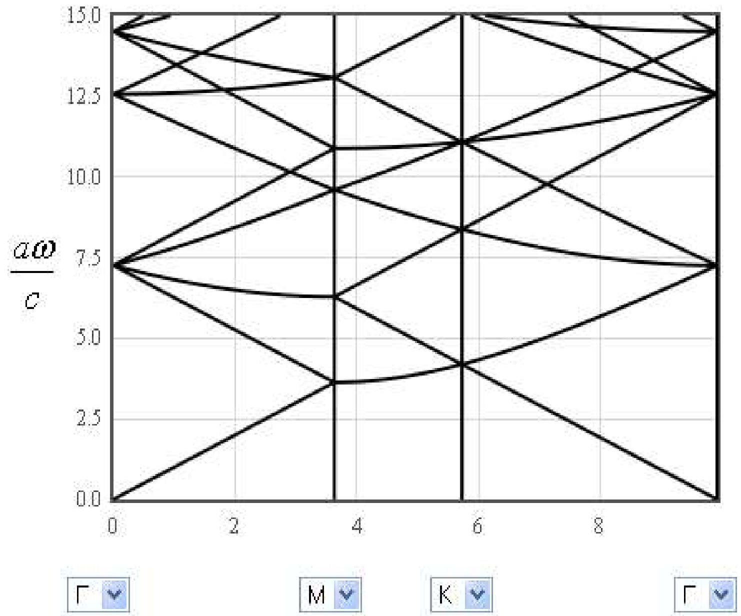


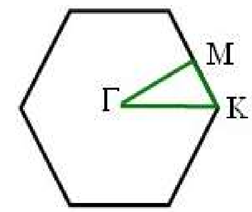


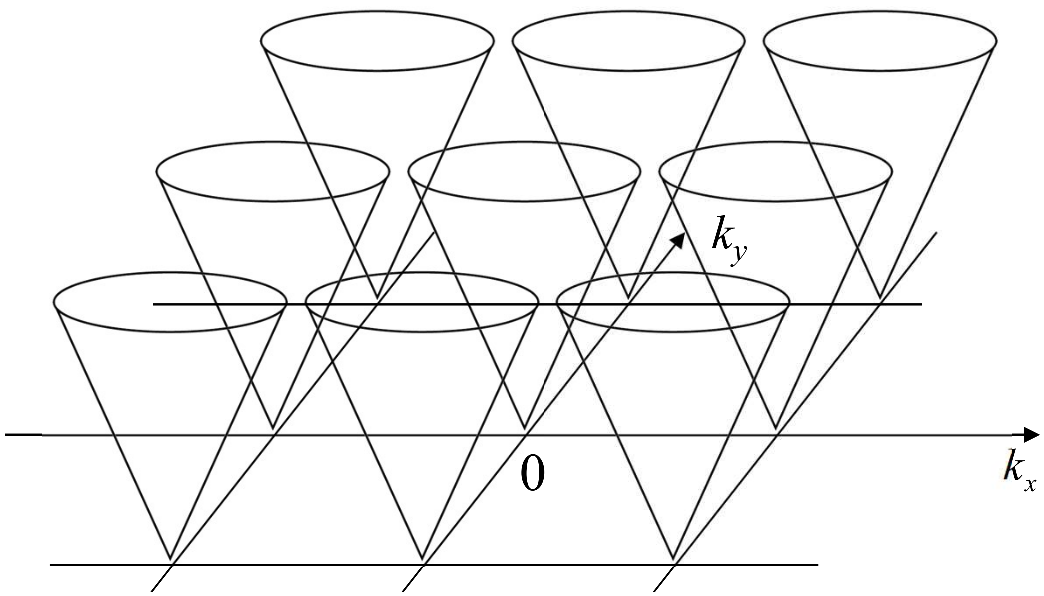
Empty lattice approximation

Plane wave method



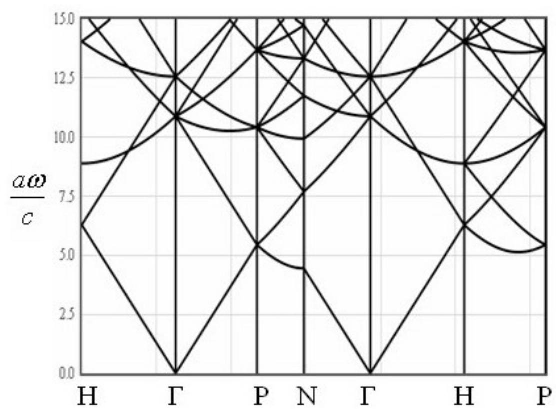




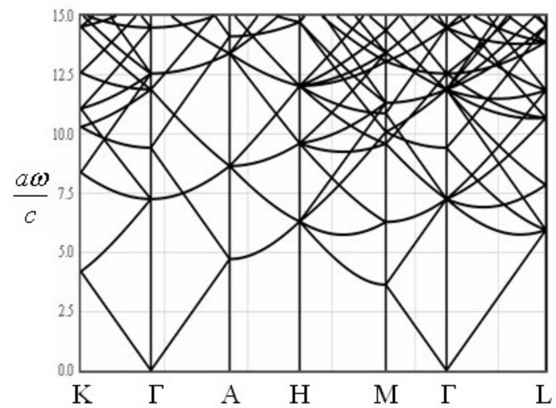


Empty lattice approximation

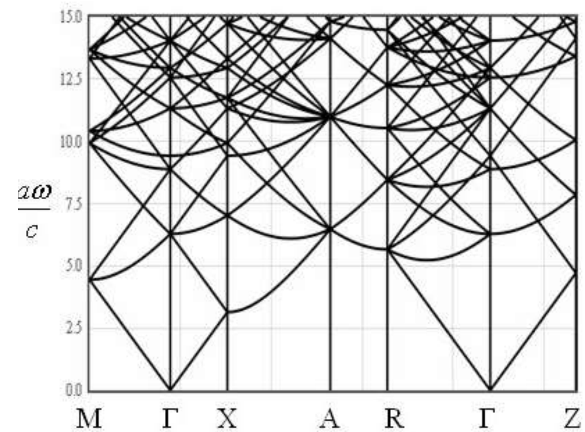
Body centered cubic

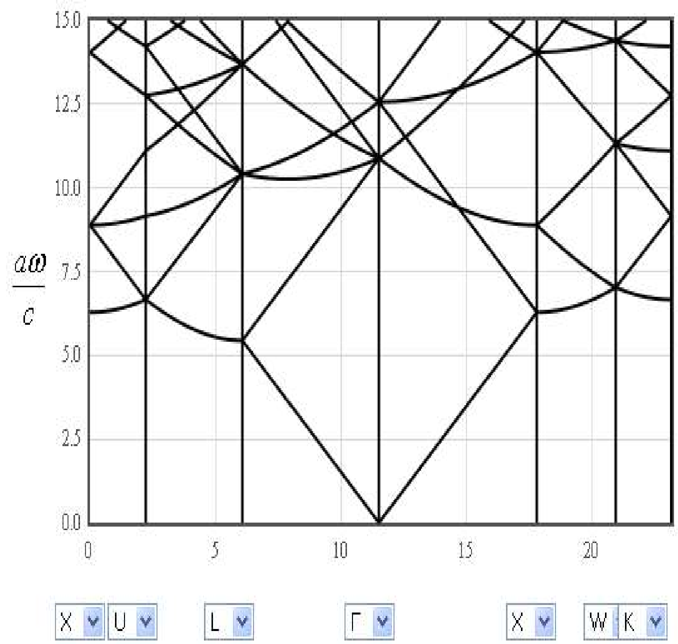


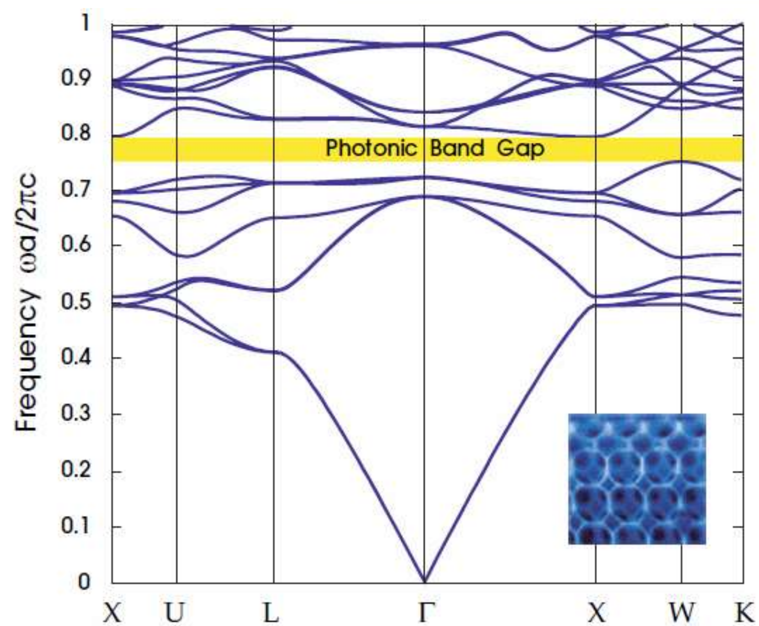
Hexagonal



Tetragonal





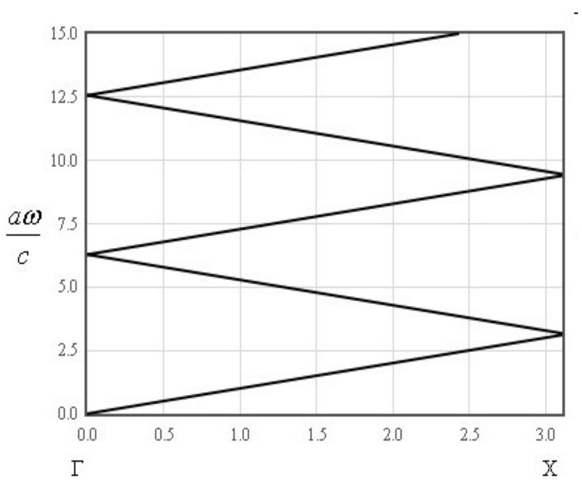


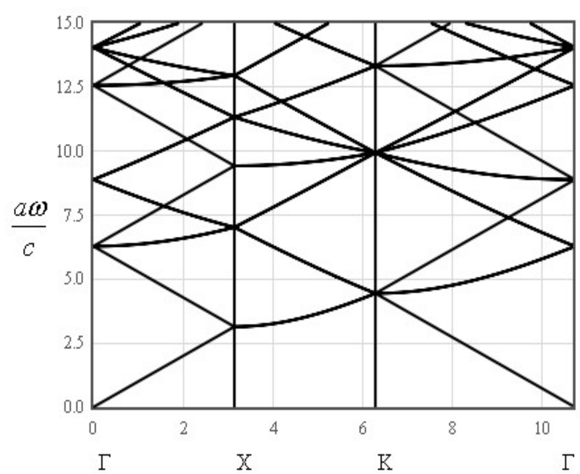
Student projects

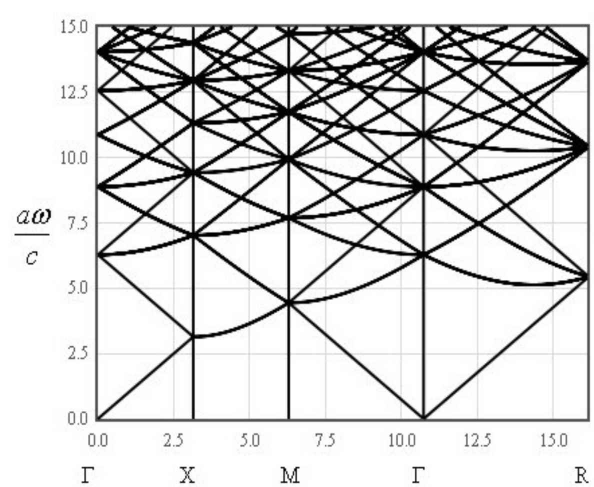
Use the plane wave method to calculate the dispersion relation for light in a 1-D layered material (or a 2-D or 3-D material)

Help complete the table of the empty lattice approximation

Write a program that will find the solutions of any second order linear differential equation with periodic coefficients





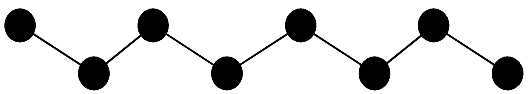


Lattice vibrations / Phonons

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

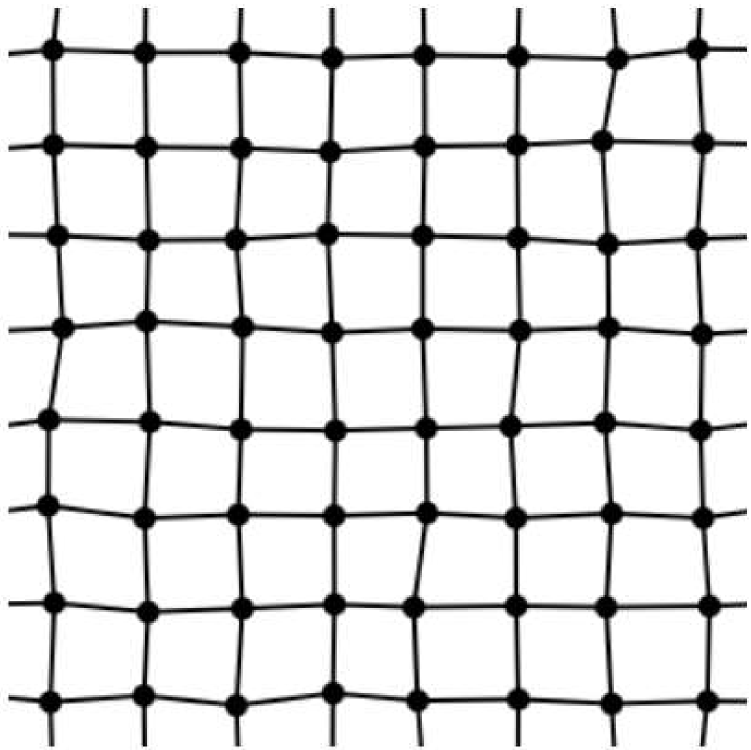
Find the phonon density of states

Calculate the thermodynamic properties

Menu | Sections | **PHY.F20 Molecular and Solid State Physics**

Normal Modes and Phonons

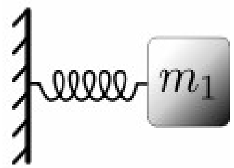
At finite temperatures, the atoms in a crystal vibrate. In the simulation below, the atoms move randomly around their equilibrium positions.



T = 300 K - +

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

Vibrations of a mass on a spring



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

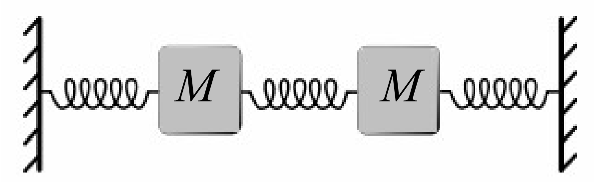
The solution has the form

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

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

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

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

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

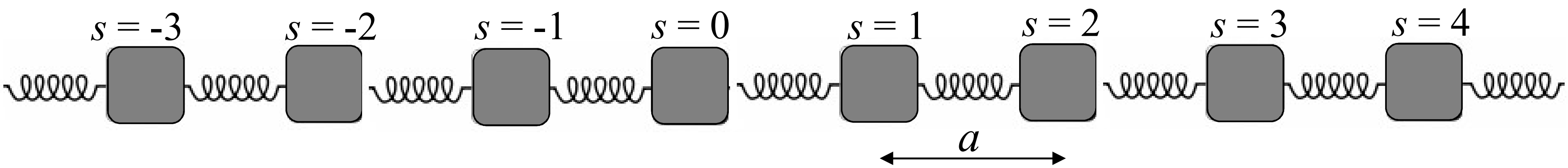
$$-\omega^2 MA_1e^{i\omega t} = -2CA_1e^{i\omega t} + CA_2e^{i\omega t}$$
$$-\omega^2 MA_2e^{i\omega t} = -2CA_2e^{i\omega t} + CA_1e^{i\omega t}$$

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

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

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

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

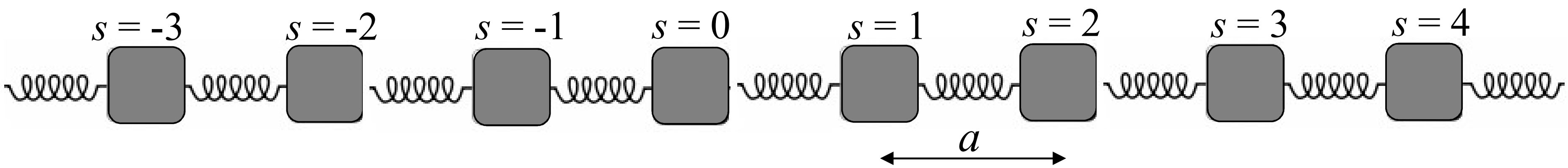
Eigen vectors of the translation operator

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

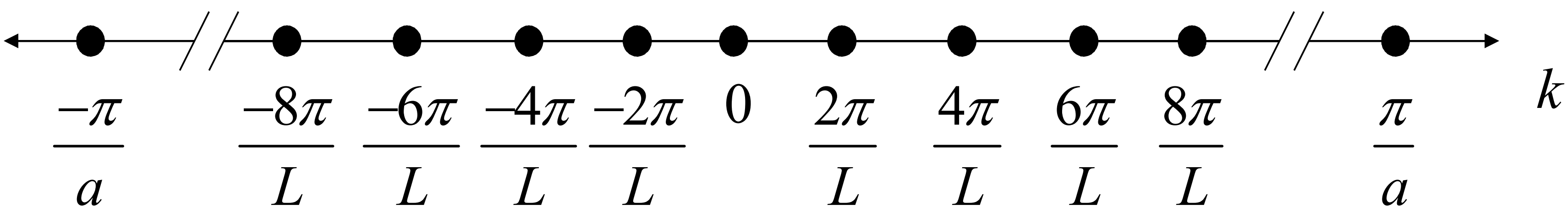
$$\begin{bmatrix} 1 \\ e^{i2\pi j/N} \\ e^{i4\pi j/N} \\ e^{i4\pi j/N} \\ \vdots \\ e^{i2\pi (N-1) j/N} \end{bmatrix} \qquad j = 1, \cdots, N$$

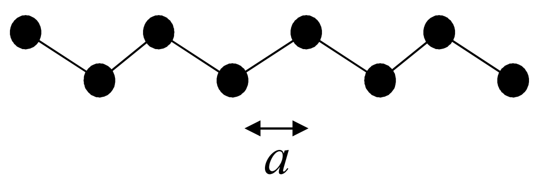
$$\begin{bmatrix} 1 \\ e^{ika} \\ e^{i2ka} \\ e^{i3ka} \\ \vdots \\ e^{-ika} \end{bmatrix} \qquad k = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \cdots$$

Linear Chain

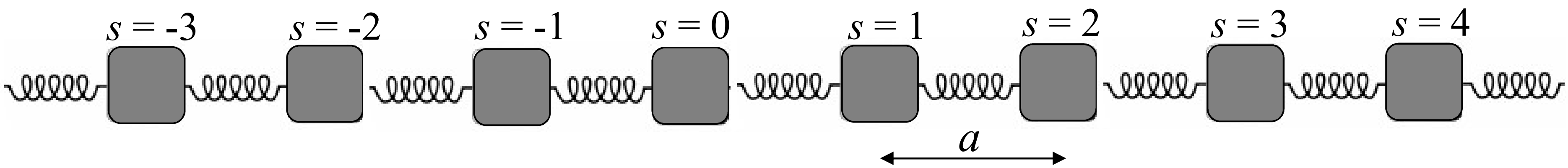


solution: $$u_s = A_k e^{i(ksa - \omega t)} = A_k e^{iksa} e^{-i\omega t}$$





Normal modes are eigen functions of T



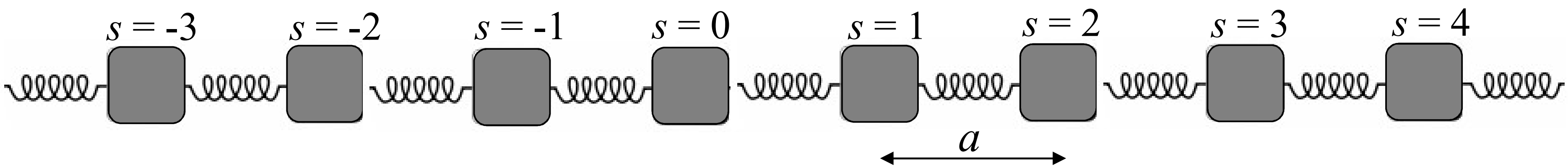
solutions are eigenfunctions of the translation operator

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

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

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

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

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

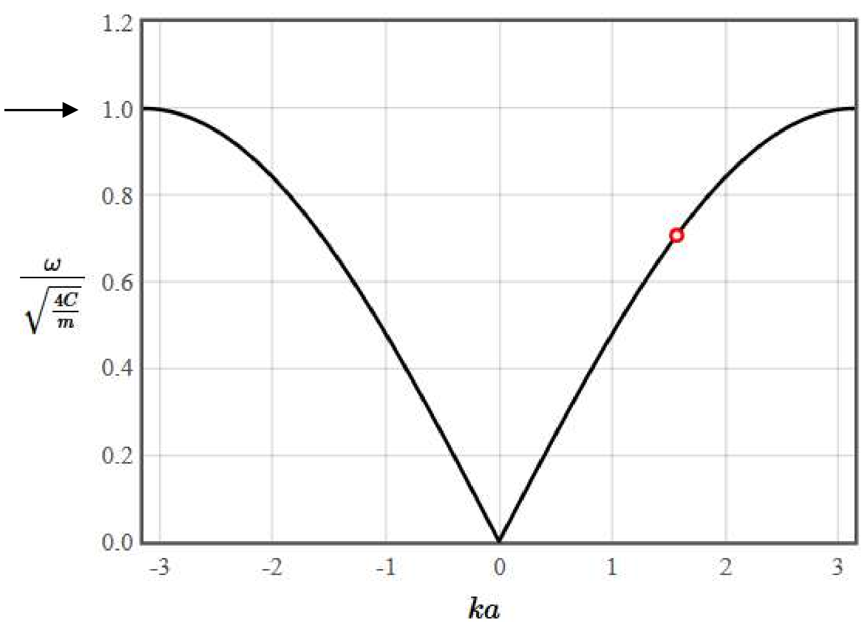
$$\omega^2 m = 2C(1-\cos(ka))$$

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

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

Linear Chain - dispersion relation

Max. freq. →



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

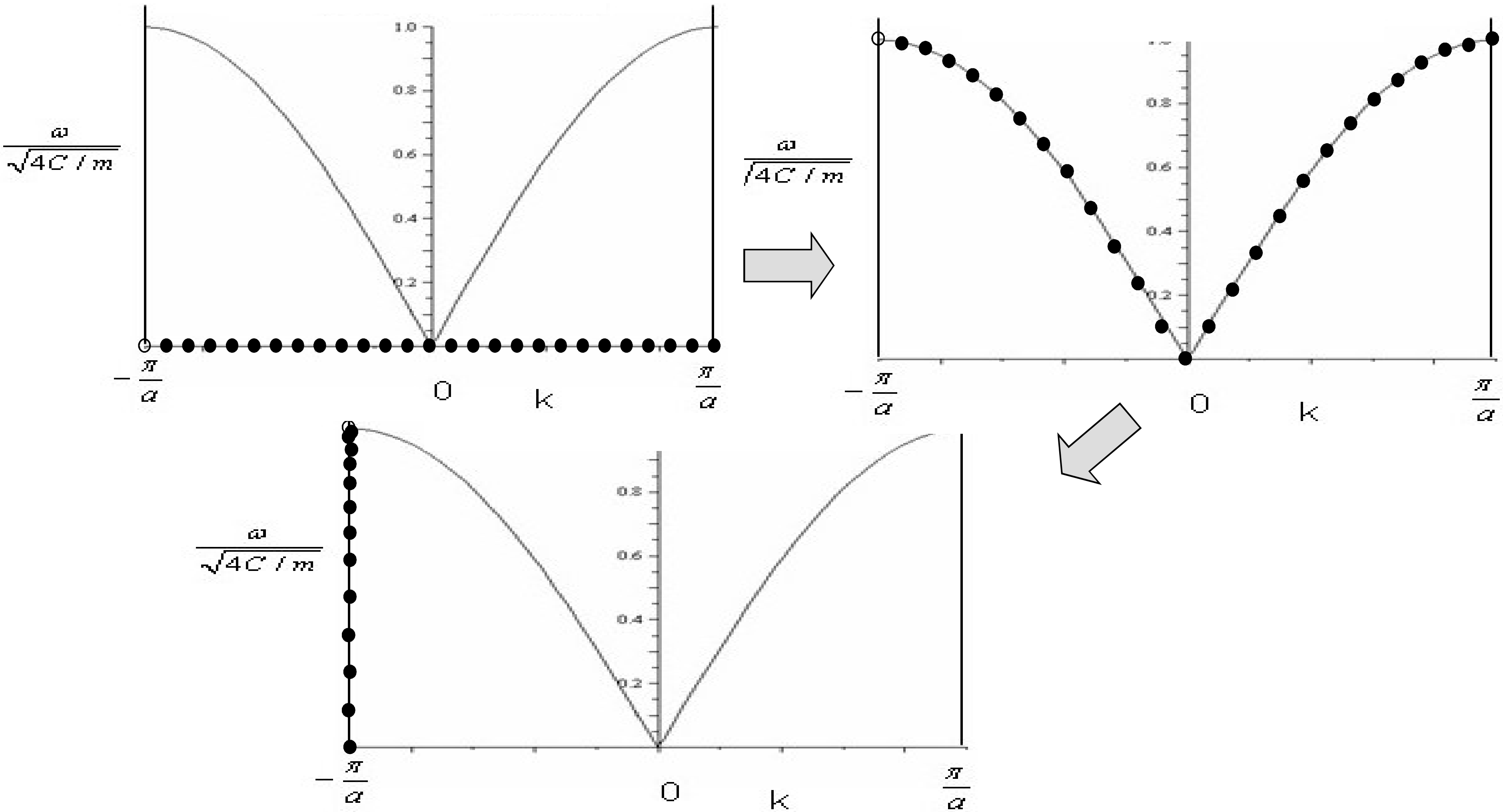
$$u_s = A_k e^{i(ksa-\omega t)}$$

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

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

Linear Chain - density of states

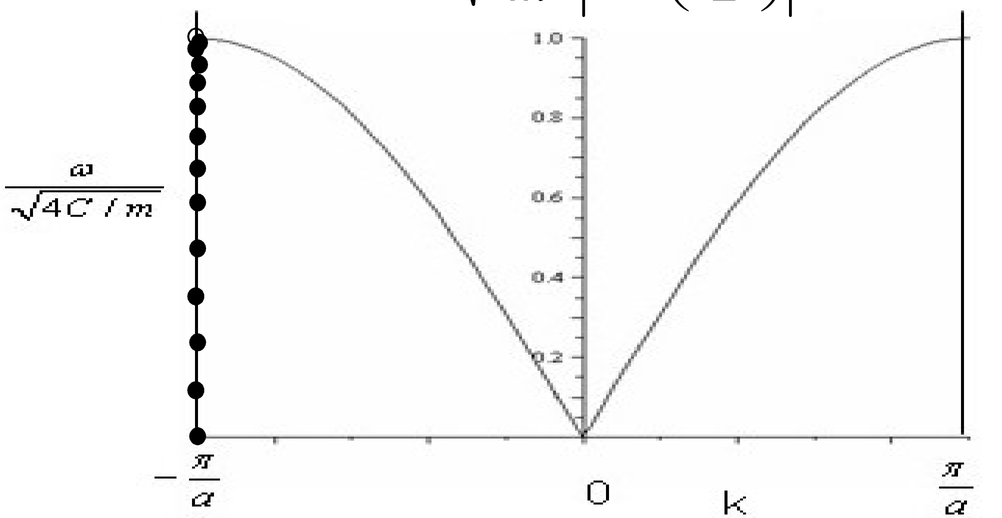
Determine the density of states numerically $\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$



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

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

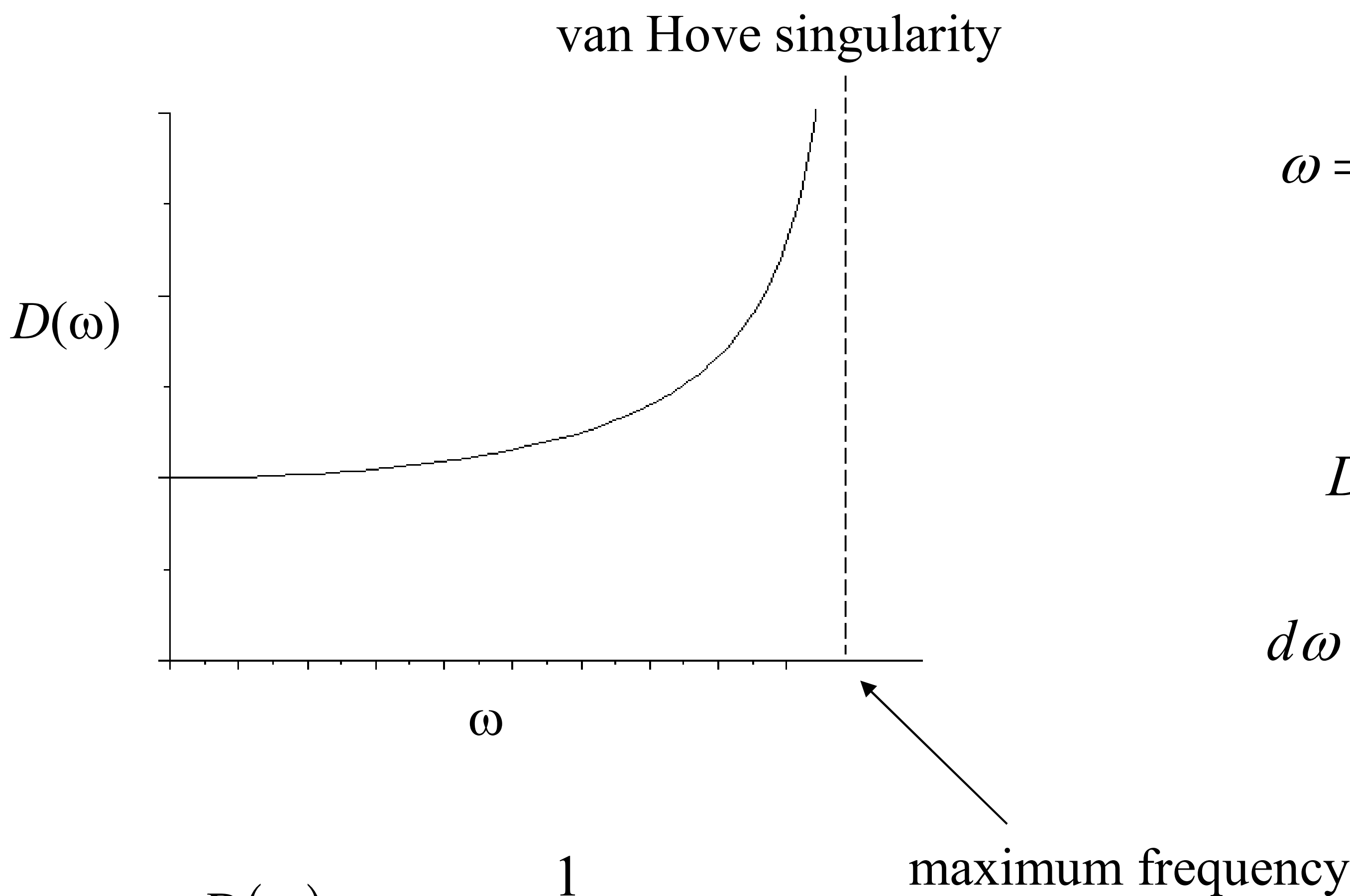
$$D(k) = \frac{1}{\pi}$$

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

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

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

density of states



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

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

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

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

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

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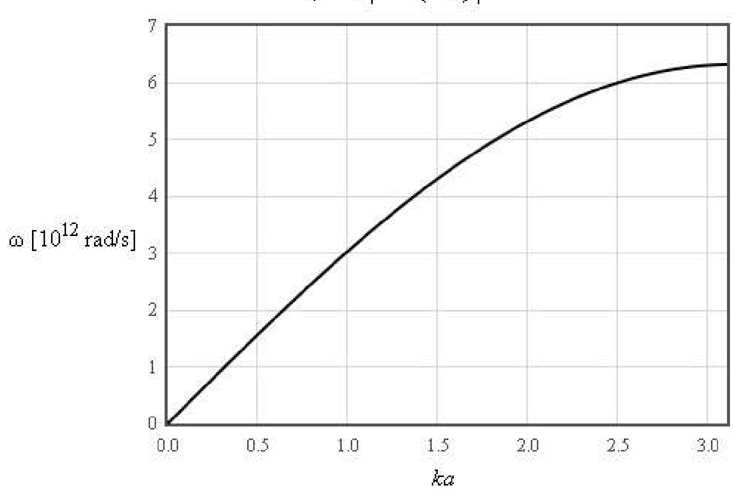
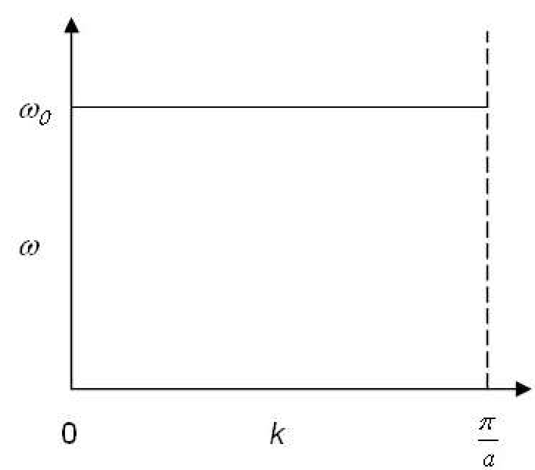
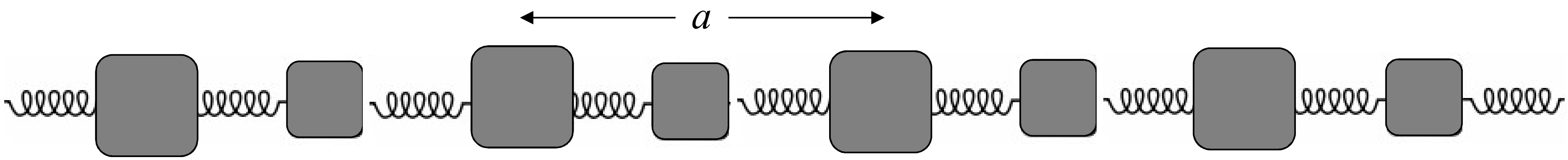
Phonons

	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

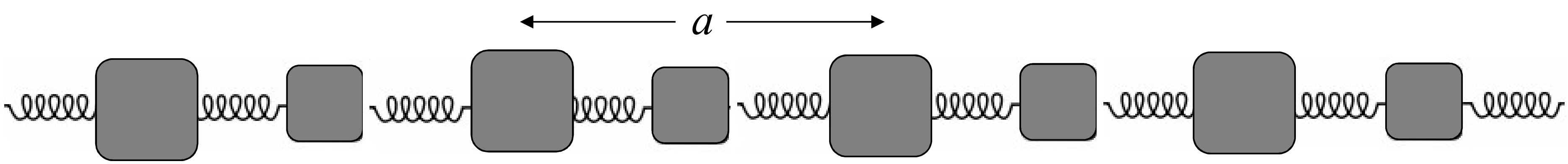
$$u_s = u_k e^{i(ksa - \omega t)}$$

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

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

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

Linear chain M_1 and M_2



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

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

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

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

dispersion relation

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