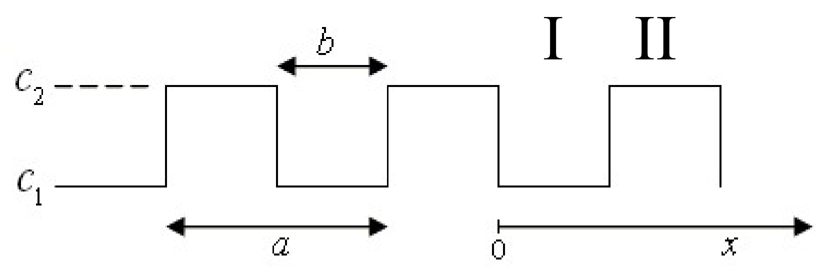
Light in a layered material



Hill's equation $$\frac{d^2\xi(x)}{dx^2} = -\frac{\omega^2}{c^2(x)}\xi(x)$$

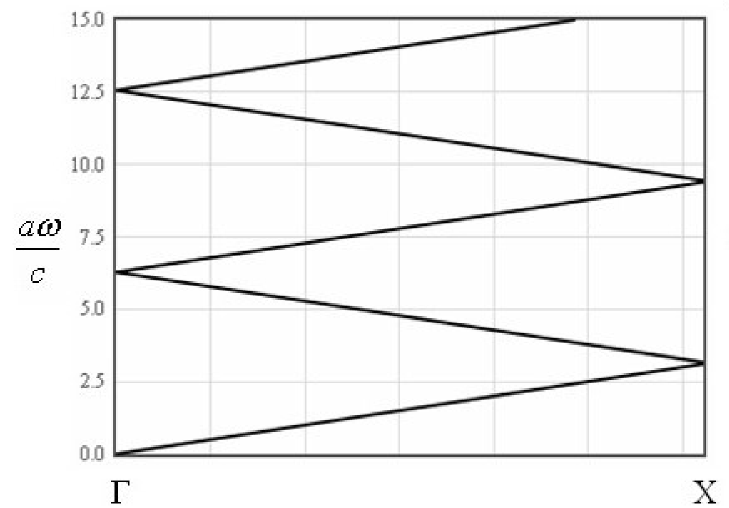
In region I, the solutions are $\sin(\omega x/c_1)$ and $\cos(\omega x/c_1)$.

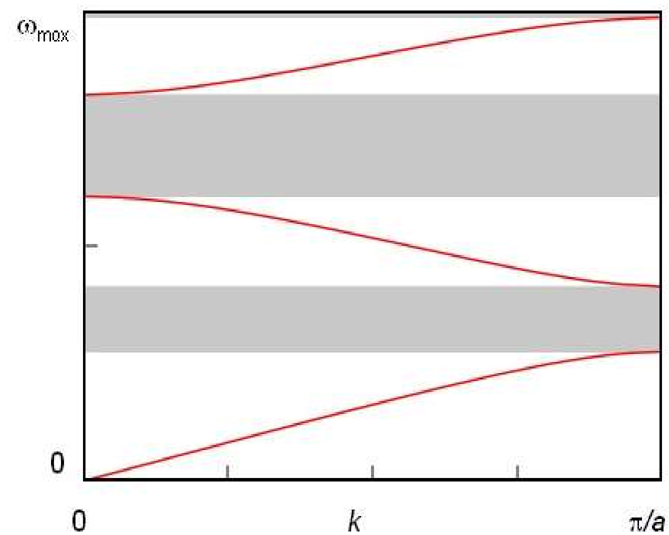
In region II, the solutions are $\sin(\omega x/c_2)$ and $\cos(\omega x/c_2)$.

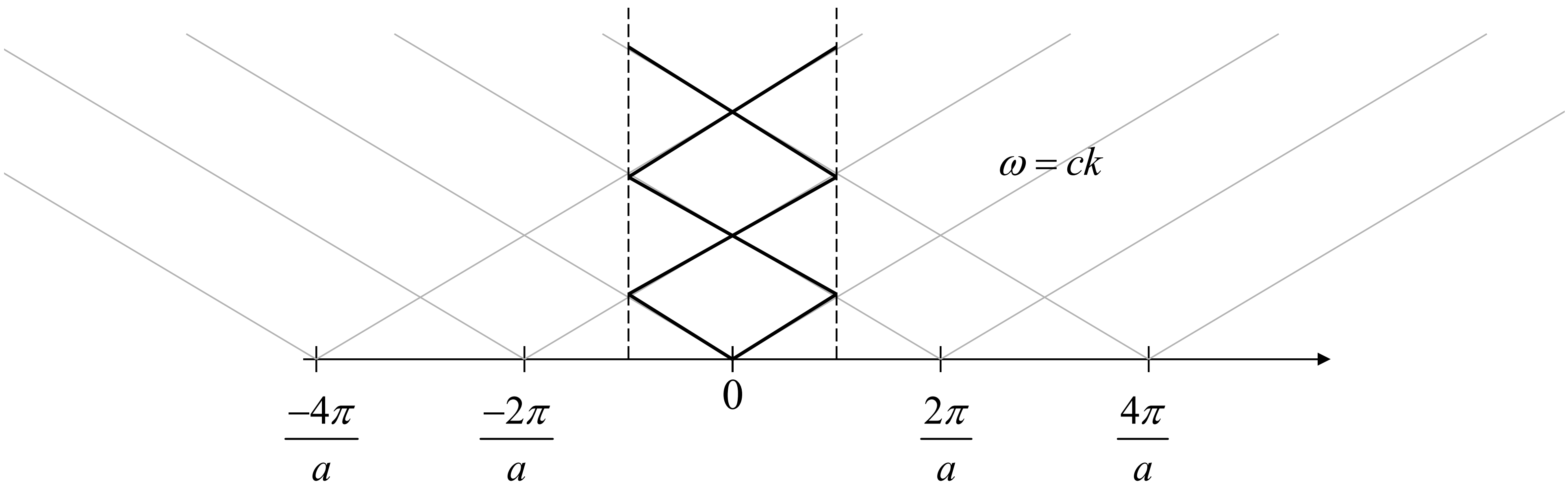
Match the solutions at the boundaries.

Normal modes don't have a clearly defined wavelength.

Empty lattice approximation

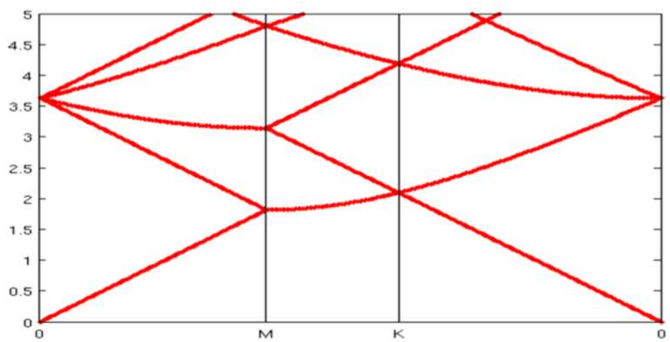


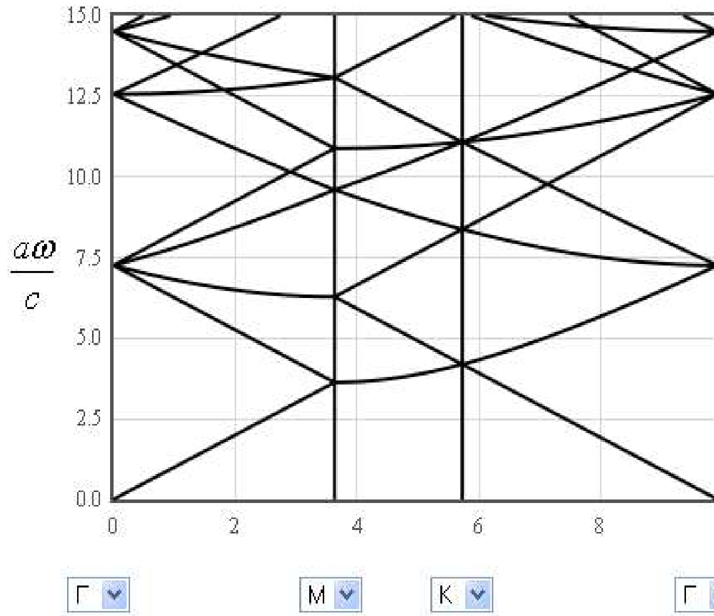


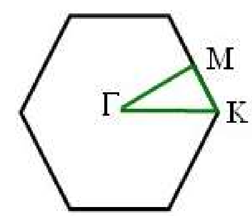


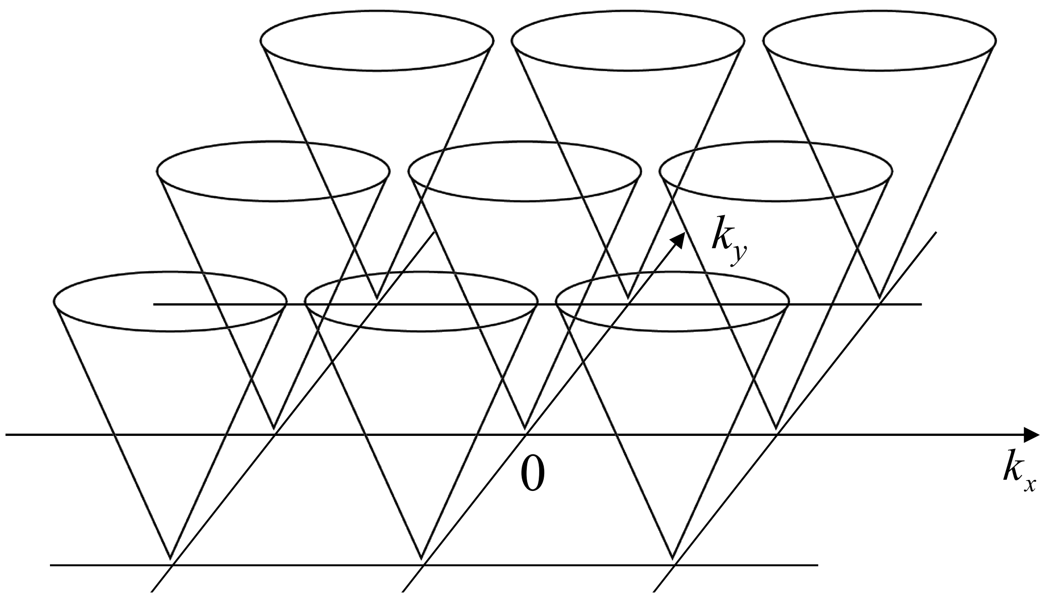
Empty lattice approximation

Plane wave method



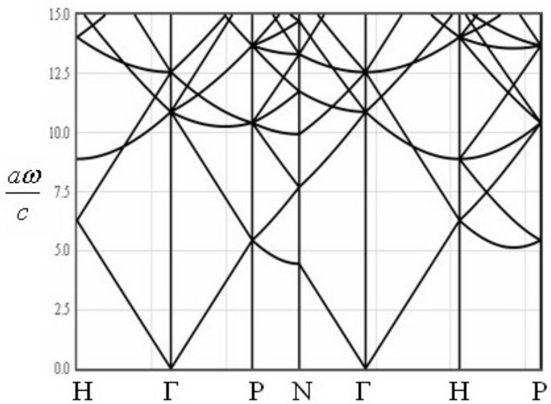




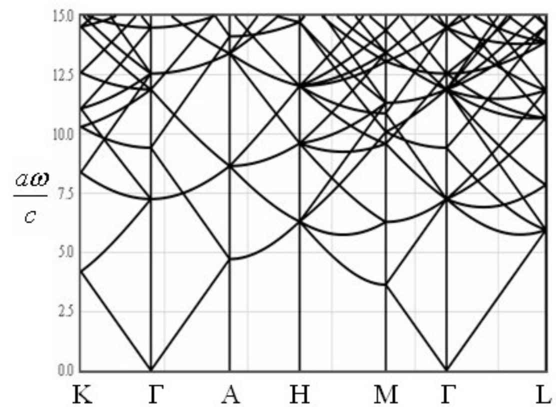


Empty lattice approximation

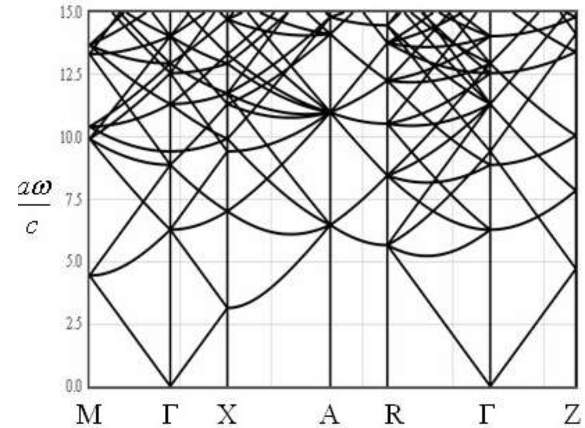
Body centered cubic

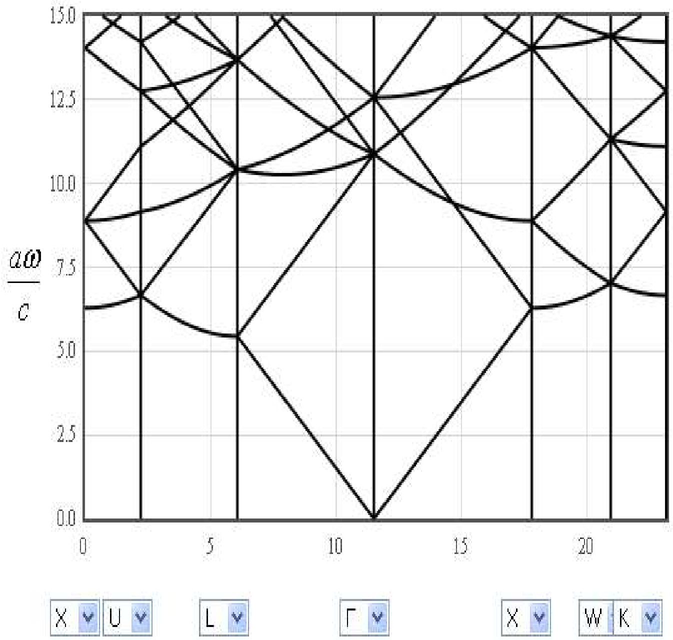


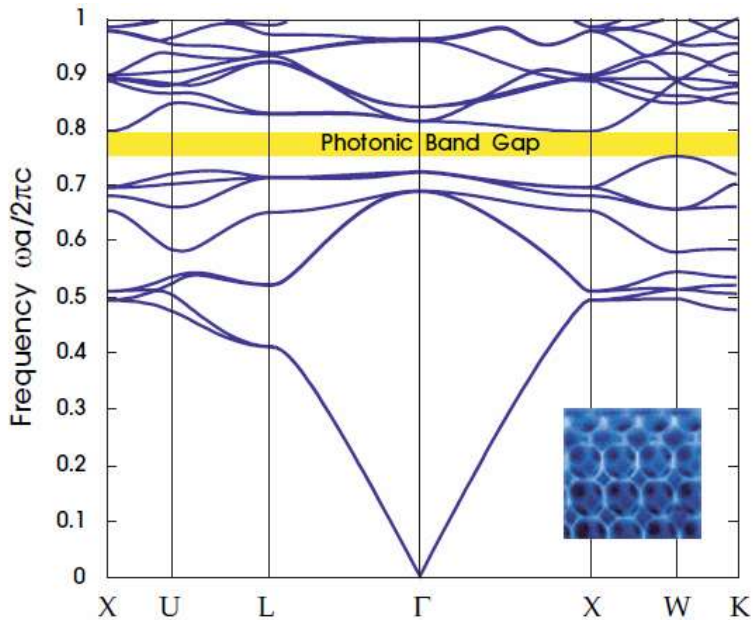
Hexagonal



Tetragonal







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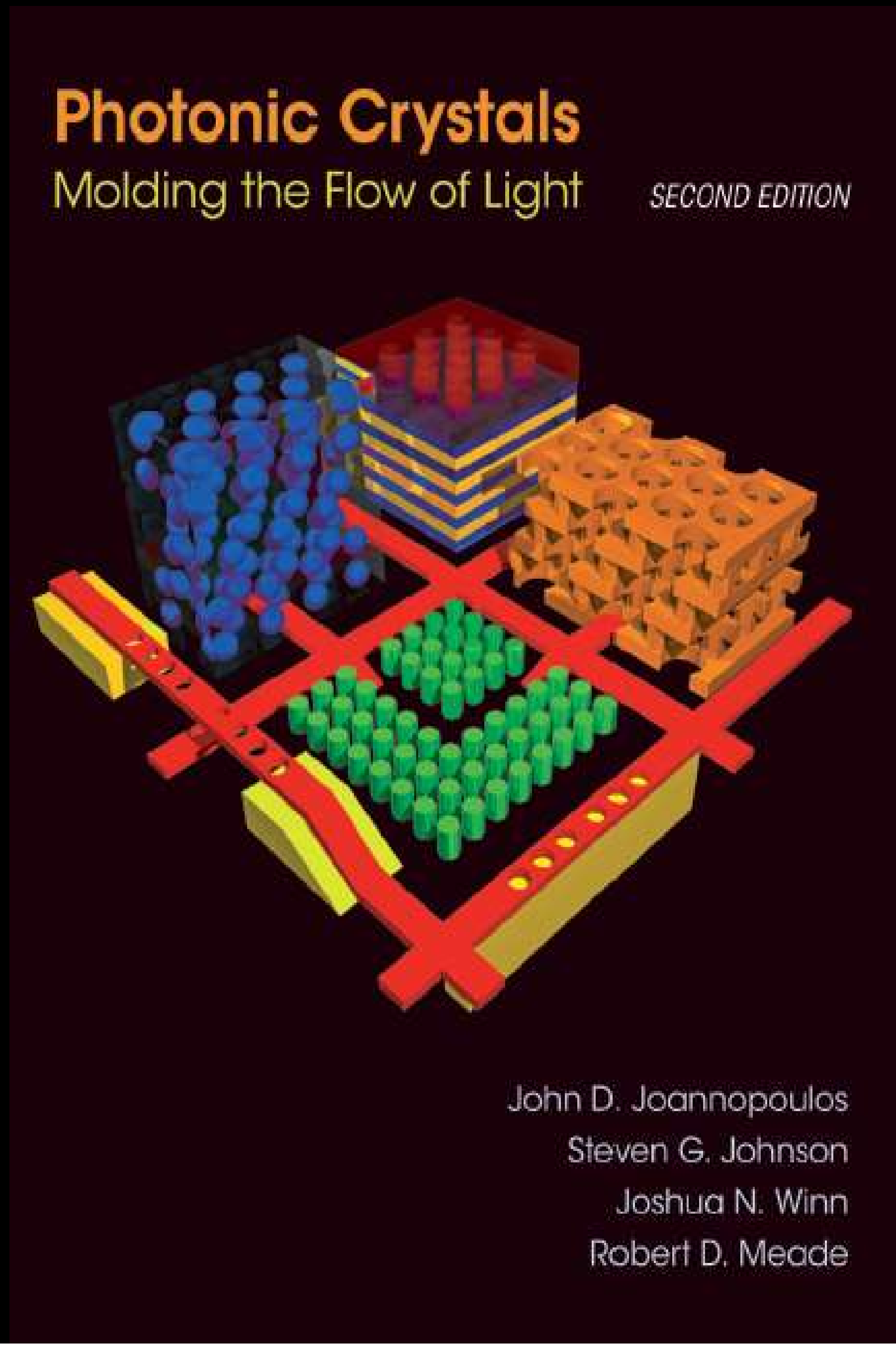
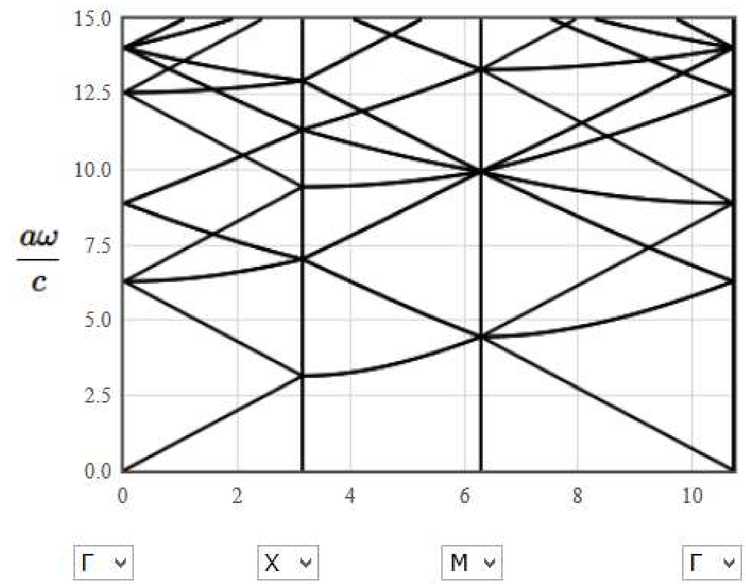
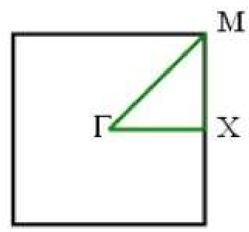
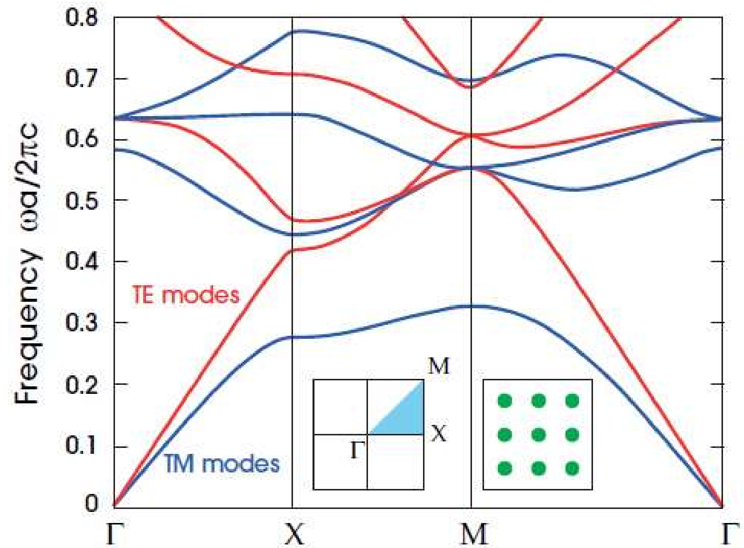


Empty lattice approximation







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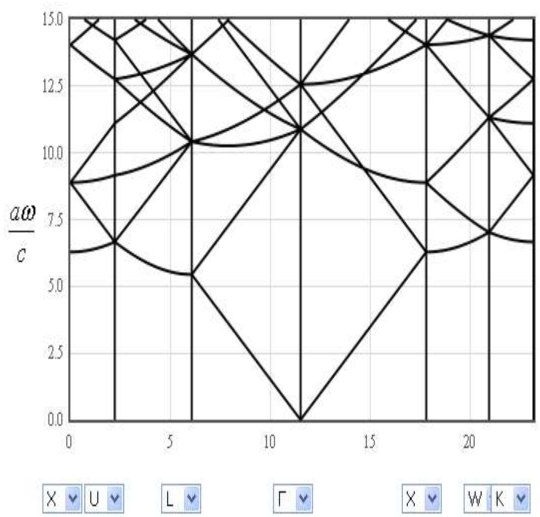
fcc



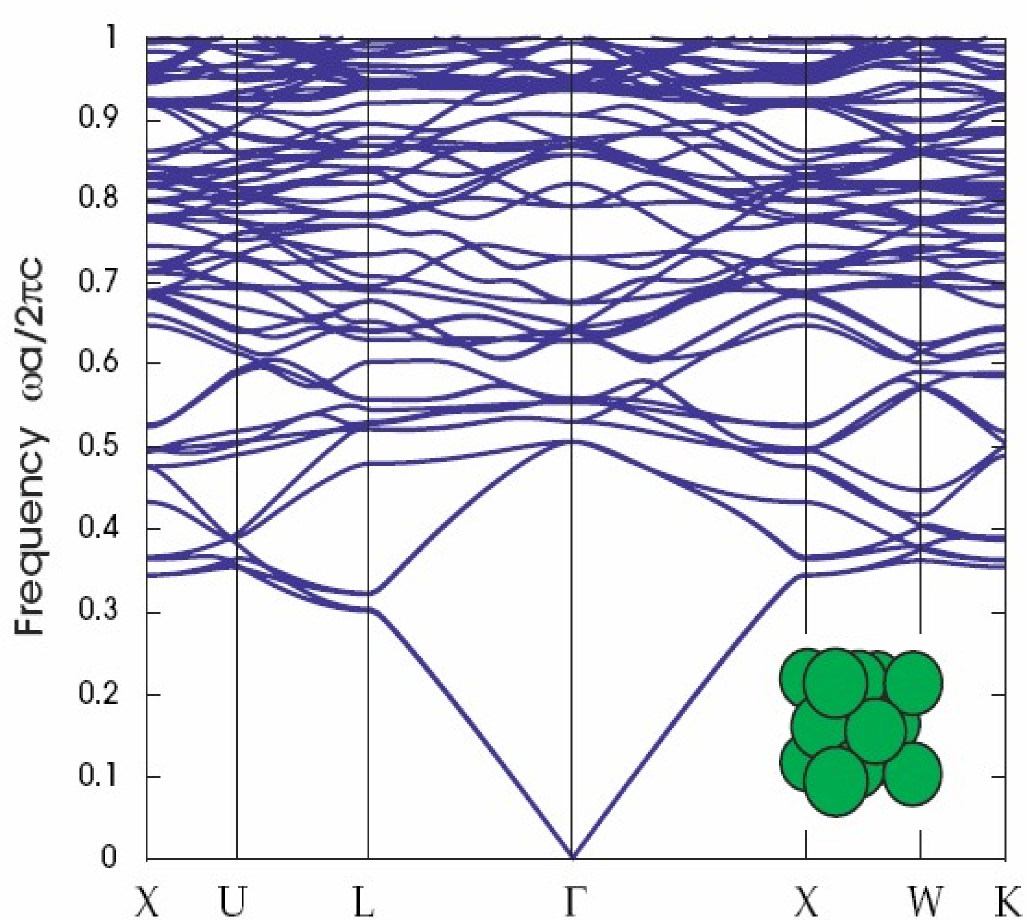


Figure 2: The photonic band structure for the lowest-frequency electromagnetic modes of a face-centered cubic (fcc) lattice of close-packed dielectric spheres ($\varepsilon = 13$) in air (inset). Note the *absence* of a complete photonic band gap. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points; see appendix B for a discussion of the Brillouin zone of an fcc lattice.

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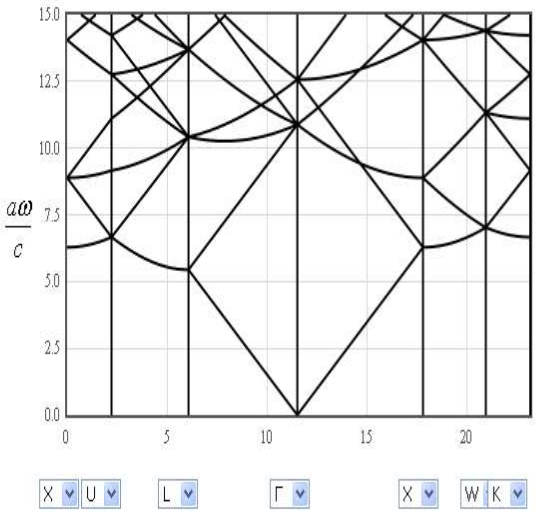
diamond



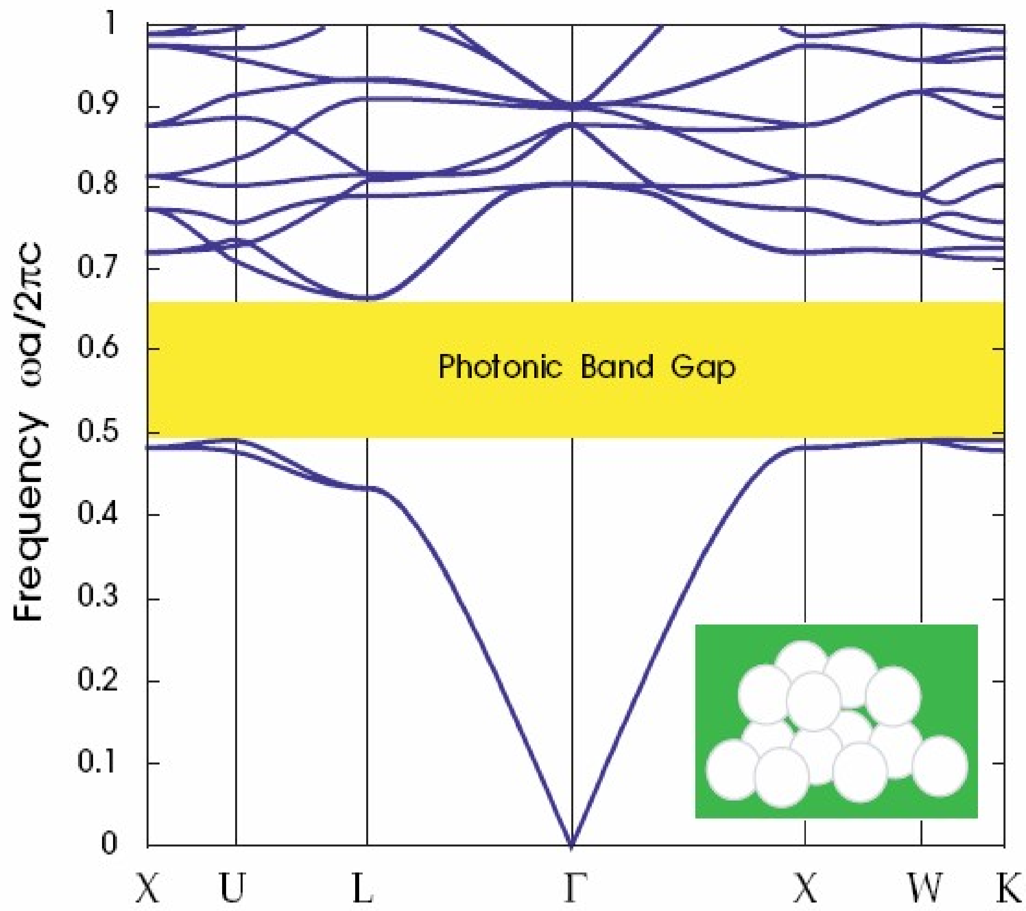


Figure 3: The photonic band structure for the lowest bands of a diamond lattice of air spheres in a high dielectric ($\varepsilon = 13$) material (inset). A complete photonic band gap is shown in yellow. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points; see appendix B for a discussion of the Brillouin zone of an fcc lattice.

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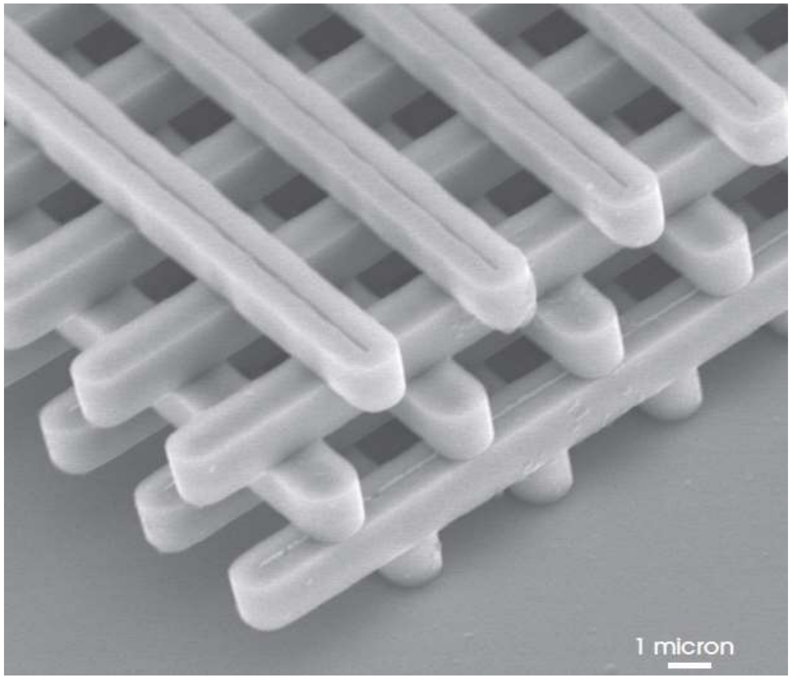
Woodpile photonic crystal



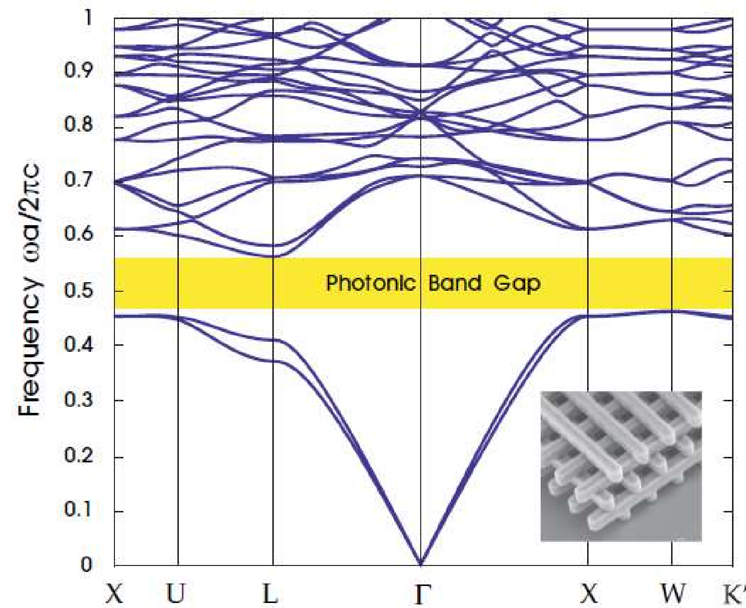
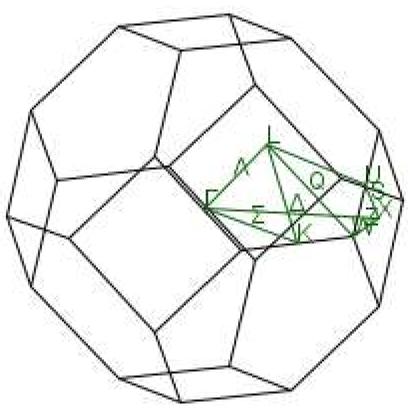


Figure 7: The photonic band structure for the lowest bands of the woodpile structure (inset, from figure 6) with $\varepsilon = 13$ logs in air. The irreducible Brillouin zone is larger than that of the fcc lattice described in appendix B, because of reduced symmetry—only a portion is shown, including the edges of the complete photonic band gap (yellow).



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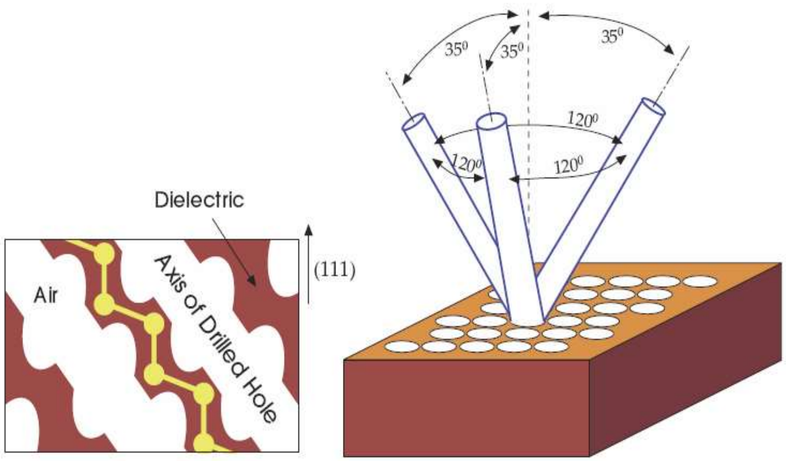
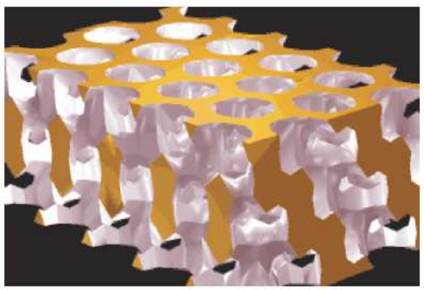
Yablonovite





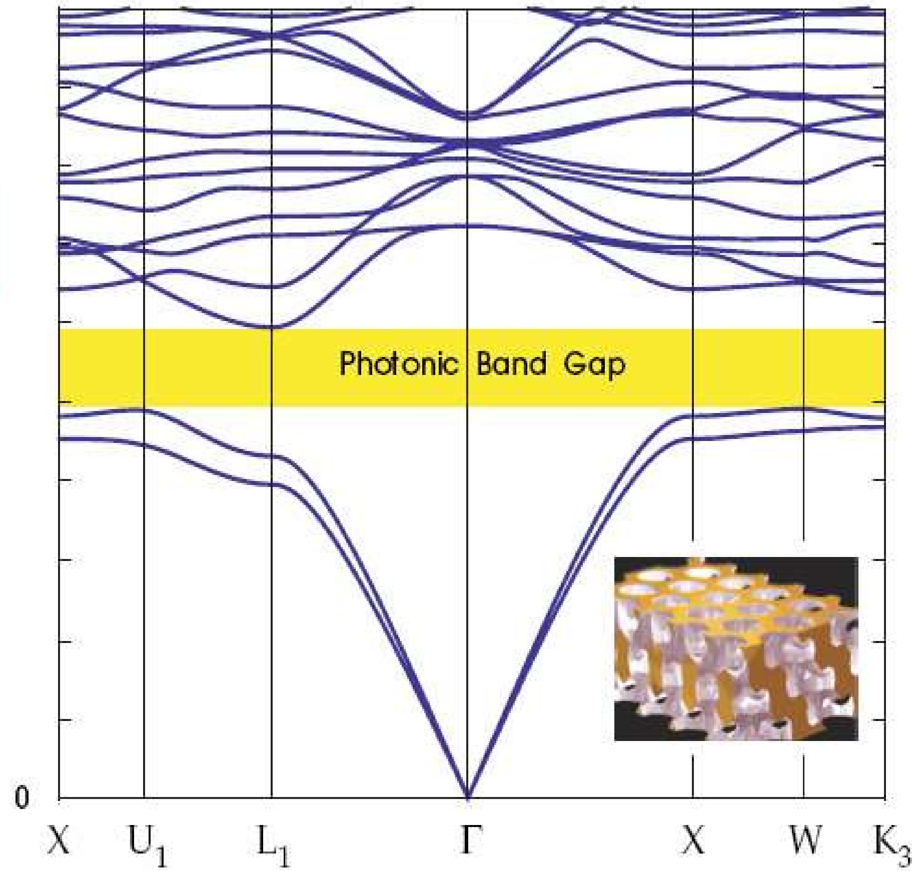


Figure 5: The photonic band structure for the lowest bands of Yablonovite (inset, from figure 4). Wave vectors are shown for a portion of the irreducible Brillouin zone that includes the edges of the complete gap (yellow). A detailed discussion of this band structure can be found in Yablonovitch et al. (1991*a*).

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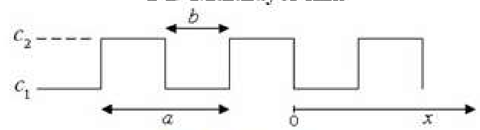
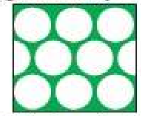
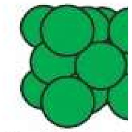
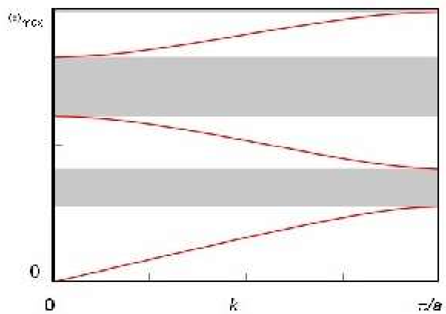
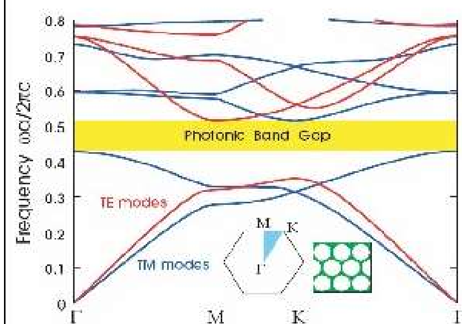
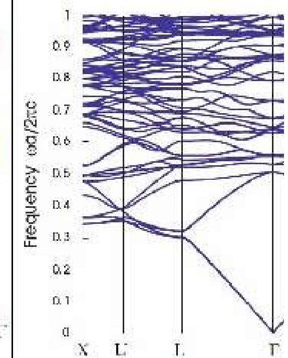
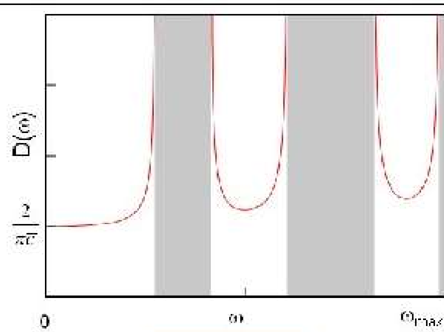
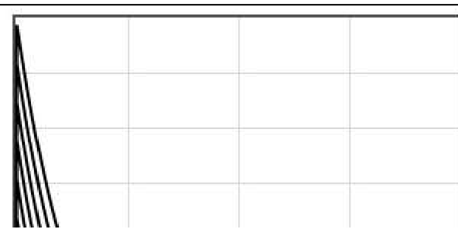
Photonic crystals

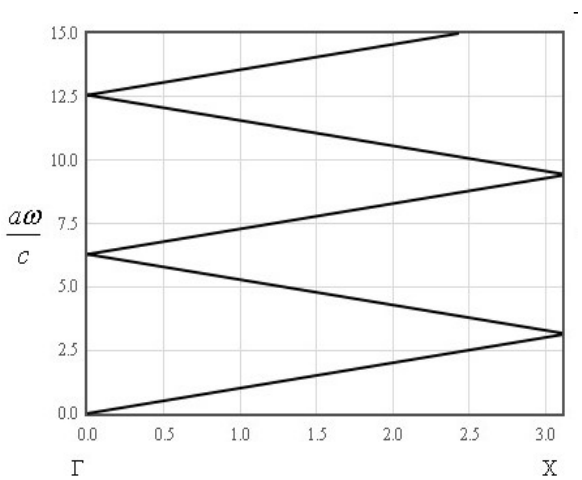
	1-D Multilayer film	2-D triangular array of air holes	fcc
	 1-D Multilayer film	 http://ab-initio.mit.edu/book	 http://ab-initio.mit.
Dispersion relation	 Calculate ω(k)	 http://ab-initio.mit.edu/book	 http://ab-initio.mit.
Density of states	 Calculate DoS		
Energy spectral density $u(\omega)=\frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_BT}\right)-1}$			

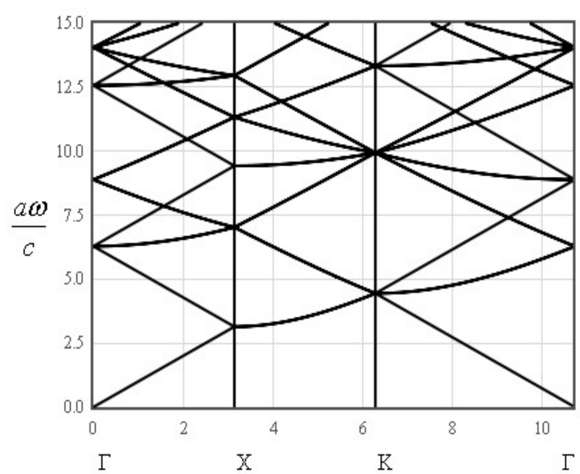
Student projects

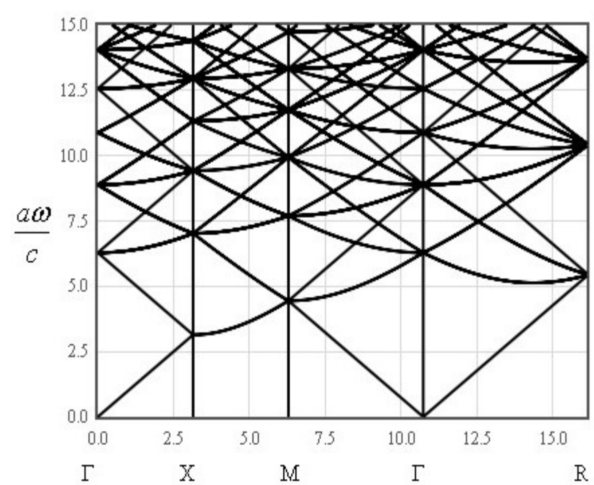
Use the plane wave method to calculate the dispersion relation for light is a 1-D layered material

Help complete the table of the empty lattice approximation

Write a program that solves Hill's equation







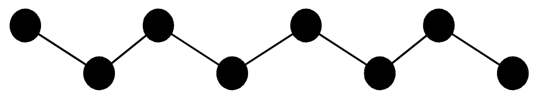
Lattice vibrations / Phonons

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

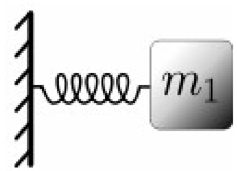


Quantize the normal modes

Find the phonon density of states

Calculate the thermodynamic properties

Vibrations of a mass on a spring



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

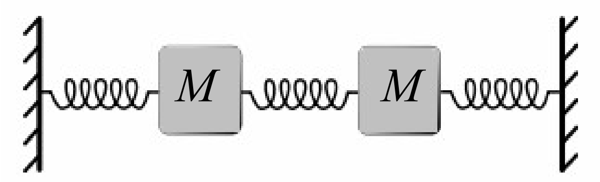
The solution has the form

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

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

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

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

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

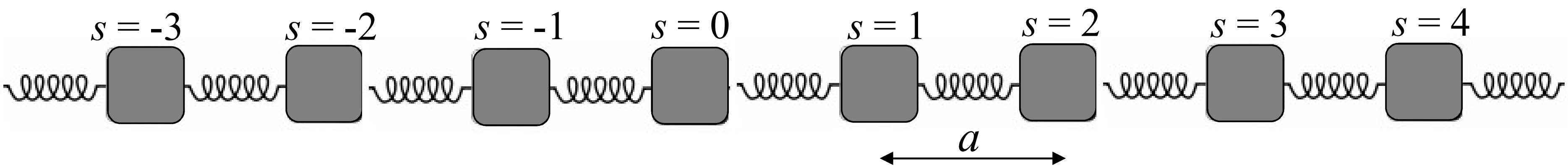
$$-\omega^2 MA_1e^{i\omega t} = -2CA_1e^{i\omega t} + CA_2e^{i\omega t}$$
$$-\omega^2 MA_2e^{i\omega t} = -2CA_2e^{i\omega t} + CA_1e^{i\omega t}$$

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

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

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

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

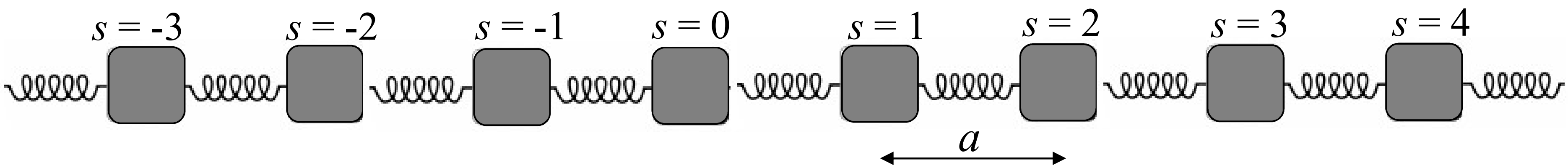
Eigen vectors of the translation operator

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

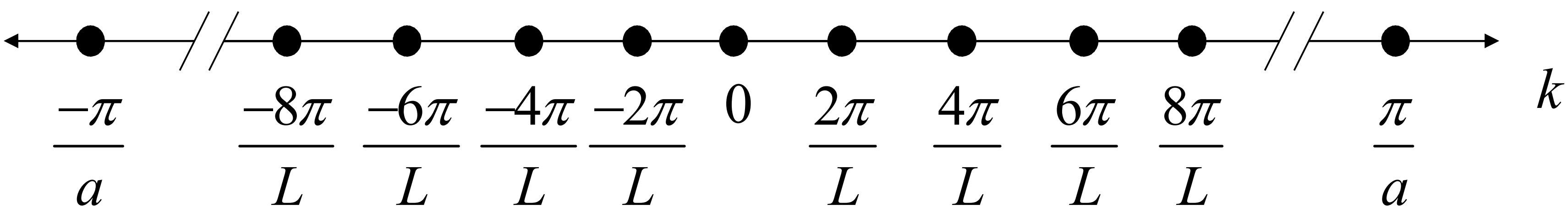
$$\begin{bmatrix} 1 \\ e^{i2\pi j/N} \\ e^{i4\pi j/N} \\ e^{i4\pi j/N} \\ \vdots \\ e^{i2\pi(N-1)j/N} \end{bmatrix} \quad j = 1, \cdots, N$$

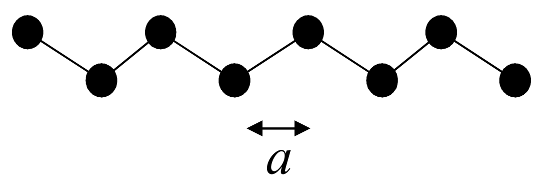
$$\begin{bmatrix} 1 \\ e^{ika} \\ e^{i2ka} \\ e^{i3ka} \\ \vdots \\ e^{-ika} \end{bmatrix} \quad k = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \cdots$$

Linear Chain

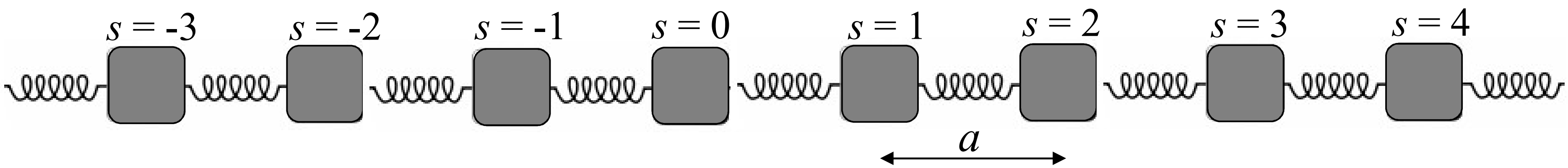


solution: $u_s = A_k e^{i(ksa-\omega t)} = A_k e^{iksa} e^{-i\omega t}$





Normal modes are eigen functions of T



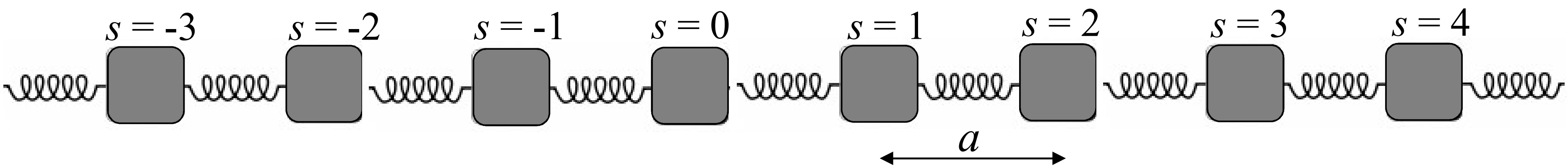
solutions are eigenfunctions of the translation operator

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

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

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

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

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

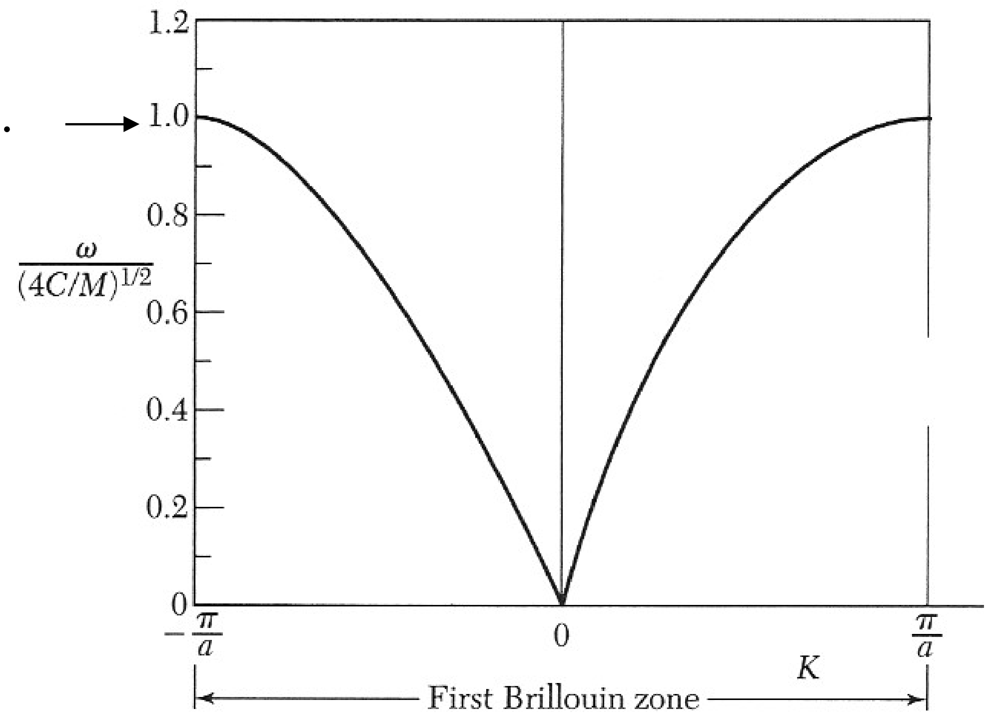
$$\omega^2 m = 2C(1-\cos(ka))$$

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

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

Linear Chain - dispersion relation

Max. freq.



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

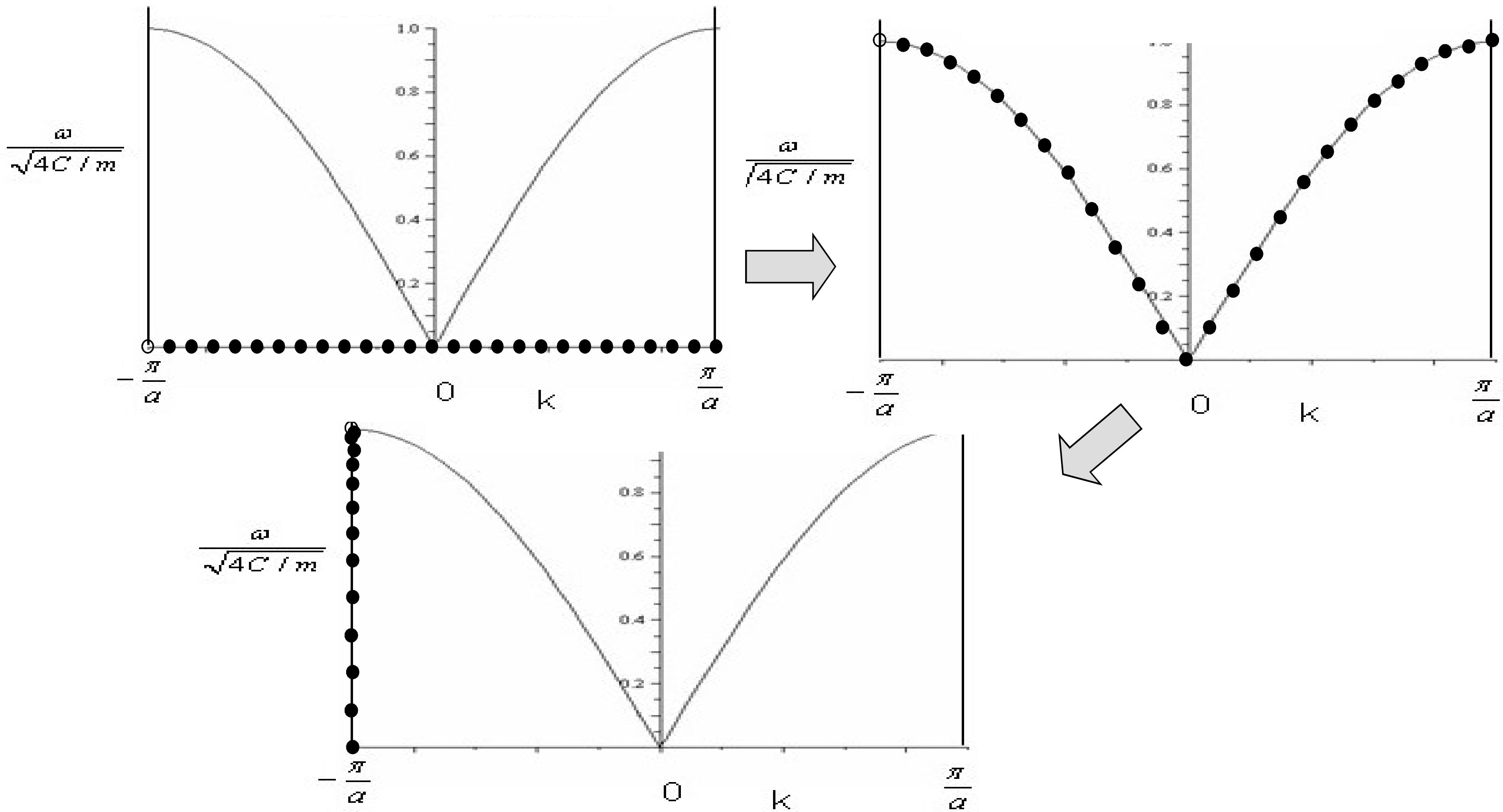
$$u_s = A_k e^{i(ksa - \omega t)}$$

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

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

Linear Chain - density of states

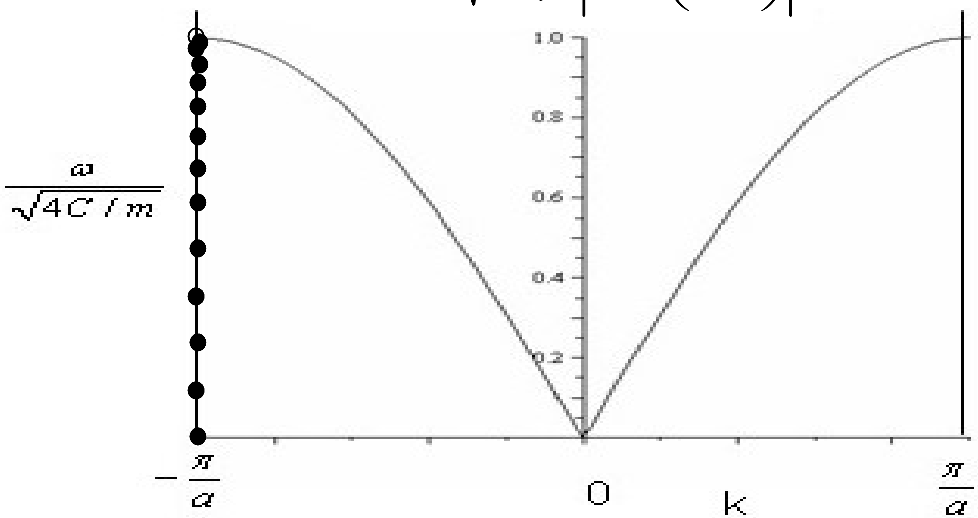
Determine the density of states numerically $\omega = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$



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

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

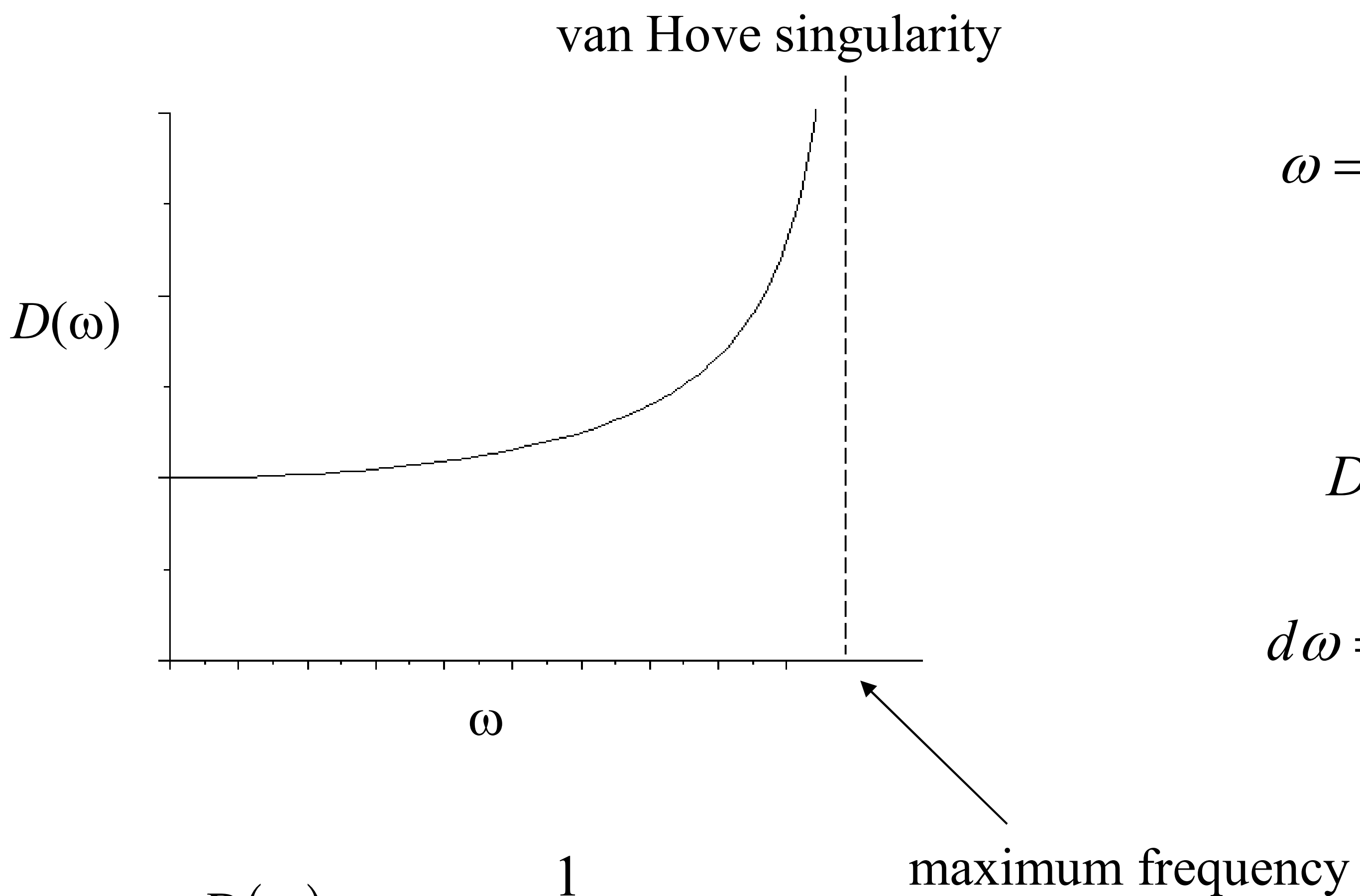
$$D(k) = \frac{1}{\pi}$$

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

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

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

density of states



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

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

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

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

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

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-of go to zero. The c
Eigenfunction solutions	$$u_s=A_ke^{i(ksa-\omega t)}$$		
Dispersion relation	$$\omega=\sqrt{\frac{4C}{m}}\left\lvert\sin\left(\frac{ka}{2}\right)\right\rvert$$