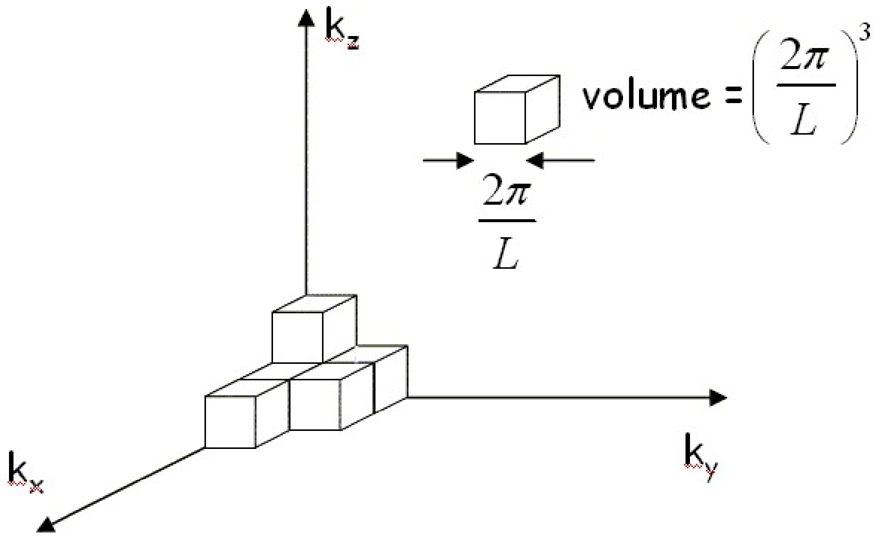
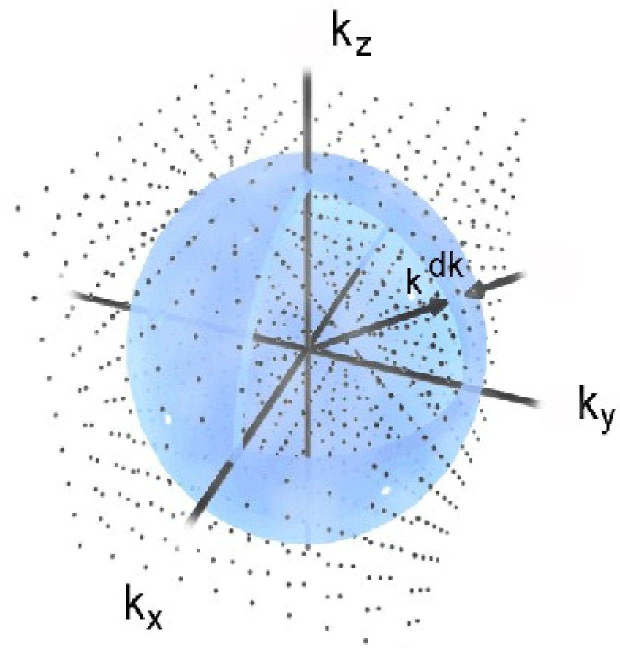
Photons

Density of states





$$k_x, k_y, k_z = \ldots, \frac{-4\pi}{L}, \frac{-2\pi}{L}, 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \ldots$$

Number of states between k and $k+dk$ for a box of size L^3. =

$$2\frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3} = \frac{k^2 L^3}{\pi^2} dk = L^3 D(k) dk$$

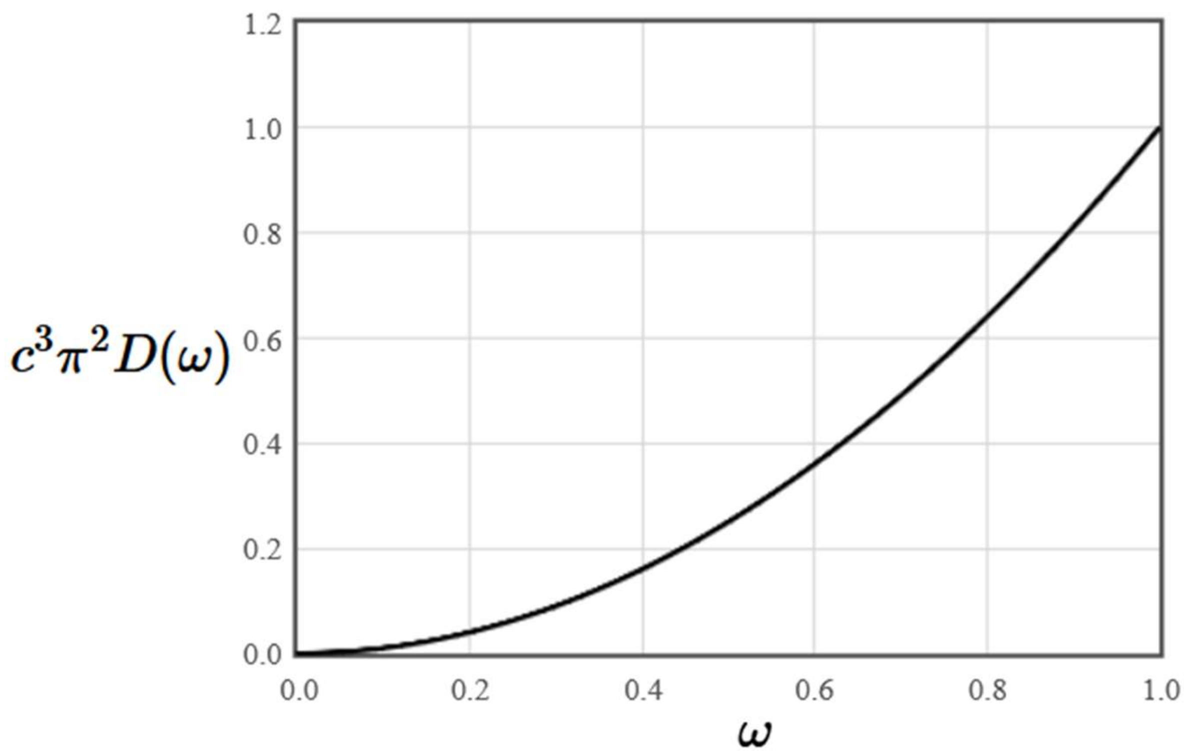
polarizations

$D(k) = k^2/\pi^2$ = density of states/m^3

Density of states

The number of states per unit volume with a frequency between ω and ω + *d*ω is,

$$D(\omega)d\omega = \frac{\omega^2}{c^3\pi^2}d\omega.$$

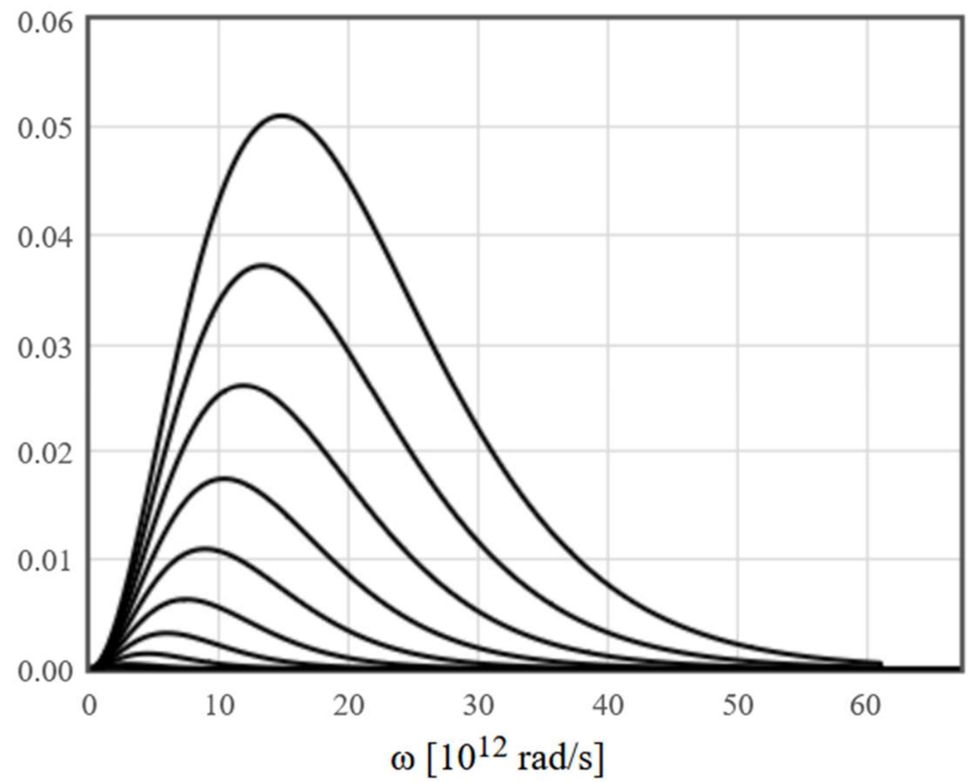


Photons are Bosons

The mean number of bosons is given by the Bose-Einstein factor.

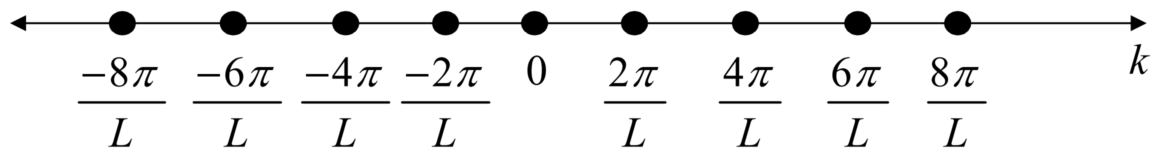
$$\frac{1}{\exp\left(\frac{\hbar\omega}{k_B T}\right)-1}$$

$$u(\omega) = \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right)-1}$$



Density of states

1-D



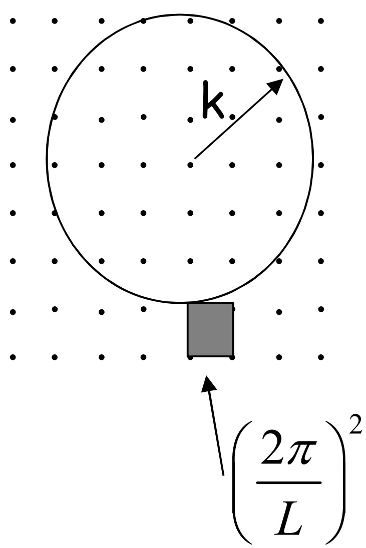
Number of states
between $|k|$ and $|k|+dk$ = $LD(k)dk = 2 \cdot 2 \cdot \frac{dk}{\frac{2\pi}{L}}$
for a line of size L.

polarizations

+/- k

$$D(k) = \frac{2}{\pi}$$

2-D

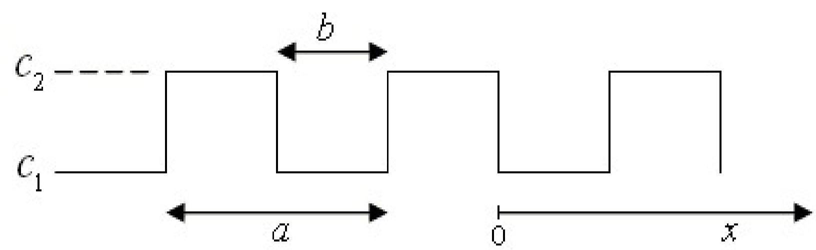


Number of states
between $|k|$ and $|k|+dk$ = $L^2 D(k)dk = 2\frac{2\pi k\ dk}{\left(\frac{2\pi}{L}\right)^2}$
for an area of size L^2.

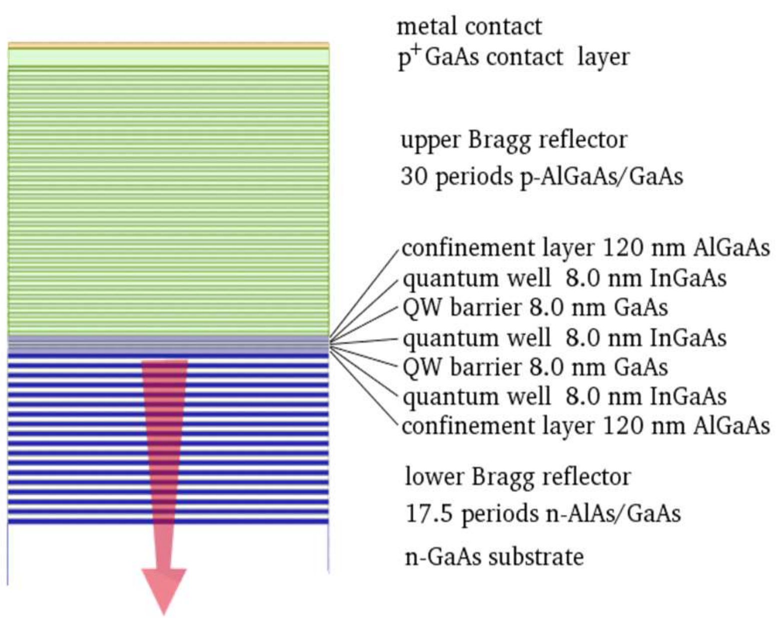
$$D(k) = \frac{k}{\pi} \qquad [\mathrm{m}^{-1}]$$

	1-D	2-D	3-D
Wave Equation c = speed of light A_j = j^{th} component of the vector potential	$c^2\frac{d^2A_j}{dx^2}=\frac{d^2A_j}{dt^2}$	$c^2\left(\frac{d^2A_j}{dx^2}+\frac{d^2A_j}{dy^2}\right)=\frac{d^2A_j}{dt^2}$	$c^2\left(\frac{d^2A_j}{dx^2}+\frac{d^2A_j}{dy^2}+\frac{d^2A_j}{dz^2}\right)=\frac{d^2A_j}{dt^2}$
Eigenfunction solutions k = wavenumber ω = angular frequency	$A_j=\exp\left(i\left(kx-\omega t\right)\right)$	$A_j=\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$	$A_j=\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$
Dispersion relation	$\omega=ck$	$\omega=c\left\|\vec{k}\right\|$	$\omega=c\left\|\vec{k}\right\|$
Density of states	$D(k)=\frac{2}{\pi}$	$D(k)=\frac{k}{\pi}$ [m^{-1}]	$D(k)=\frac{k^2}{\pi^2}$ [m^{-2}]
Density of states $D(\omega)=D(k)\frac{dk}{d\omega}$	$D(\omega)=\frac{2}{\pi c}$ [s/m]	$D(\omega)=\frac{\omega}{\pi c^2}$ [s/m^2]	$D(\omega)=\frac{\omega^2}{\pi^2c^3}$ [s/m^3]
Density of states $D(\lambda)=D(k)\frac{dk}{d\lambda}$ λ = wavelength	$D(\lambda)=\frac{4}{\lambda^2}$ [m^{-2}]	$D(\lambda)=\frac{4\pi}{\lambda^3}$ [m^{-3}]	$D(\lambda)=\frac{8\pi}{\lambda^4}$ [m^{-4}]
Density of states $D(E)=D(\omega)\frac{d\omega}{dE}$	$D(E)=\frac{2}{\pi\hbar c}$ [J^{-1}m^{-1}]	$D(E)=\frac{E}{\pi\hbar^2c^2}$ [J^{-1}m^{-2}]	$D(E)=\frac{E^2}{\pi^2\hbar^3c^3}$ [J^{-1}m^{-3}]
Chemical potential	$\mu=0$	$\mu=0$	$\mu=0$
Intensity spectral density k_B = 1.3806504 × 10^{-23} [J/K] Boltzmann's constant h = 6.62606896 × 10^{-34} [J s] Planck's constant	$I(\lambda)=\frac{2hc^2}{\lambda^3\left(\exp\left(\frac{hc}{\lambda k_BT}\right)-1\right)}$ [J m^{-1}s^{-1}]	$I(\lambda)=\frac{4hc^2}{\lambda^4\left(\exp\left(\frac{hc}{\lambda k_BT}\right)-1\right)}$ [J m^{-2}s^{-1}]	$I(\lambda)=\frac{2\pi hc^2}{\lambda^5\left(\exp\left(\frac{hc}{\lambda k_BT}\right)-1\right)}$ [J m^{-3}s^{-1}]
Wien's law $\left.\frac{dI(\lambda)}{d\lambda}\right\|_{\lambda=\lambda_{max}}=0$	$\lambda_{max}=\frac{0.0050994367}{T}$ [m]	$\lambda_{max}=\frac{0.0036696984}{T}$ [m]	$\lambda_{max}=\frac{0.002897707138}{T}$ [m]
Stefan - Boltzmann law $I=\int_0^\infty I(\lambda)d\lambda$ $\zeta(3)\approx1.202$ Riemann ζ function σ = 5.67 × 10^{-8} Stefan-Boltzmann constant	$I=\frac{\pi^2k_B^{\,2}T^2}{3h}$ [J s^{-1}]	$I=\frac{8\varsigma(3)k_B^{\,3}T^3}{h^2c}$ [J m^{-1} s^{-1}]	$I=\frac{2\pi^5k_B^4T^4}{15c^2h^3}=\sigma T^4$ [J m^{-2} s^{-2}]
Internal energy distribution $u(\lambda)=\frac{hc}{\lambda}\cdot\frac{D(\lambda)}{\exp\left(\frac{hc}{\lambda k_BT}\right)-1}$	$u(\lambda)=\frac{4hc}{\lambda^3\left(\exp\left(\frac{hc}{\lambda k_BT}\right)-1\right)}$ [J/m^2]	$u(\lambda)=\frac{4\pi hc}{\lambda^4\left(\exp\left(\frac{hc}{\lambda k_BT}\right)-1\right)}$ [J/m^3]	$u(\lambda)=\frac{8\pi hc}{\lambda^5\left(\exp\left(\frac{hc}{\lambda k_BT}\right)-1\right)}$ [J/m^4]
Internal energy $u=\int_0^\infty u(\lambda)d\lambda$	$u=\frac{2\pi^2k_B^{\,2}T^2}{3hc}$ [J/m]	$u=\frac{8\varsigma(3)\pi k_B^{\,3}T^3}{h^2c^2}$ [J/m^2]	$u=\frac{4\sigma T^4}{c}$ [J/m^3]

Light in a layered material



The dielectric constant and speed of light are different for the two layers.



Distributed Bragg reflector

Light in a layered material

Wave equation in a periodic medium $$c^2(x)\frac{\partial^2 A_j}{\partial x^2}=\frac{\partial^2 A_j}{\partial t^2}$$

Separation of variables $$A_j\left(x,t\right)=\xi(x)e^{-i\omega t}$$

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

Normal modes don't have a clearly defined wavelength.

2nd order linear differential equation with periodic coefficients.
Mathematically equivalent to the time independent Schrödinger equation.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=\left(E-V(x)\right)\psi(x)$$

Differential equations

The solutions to a linear differential equation with constant coefficients,

$$a\frac{d^2y}{dx^2}+b\frac{dy}{dx}+cy=d,$$

have the form,

$$e^{\lambda x}.$$

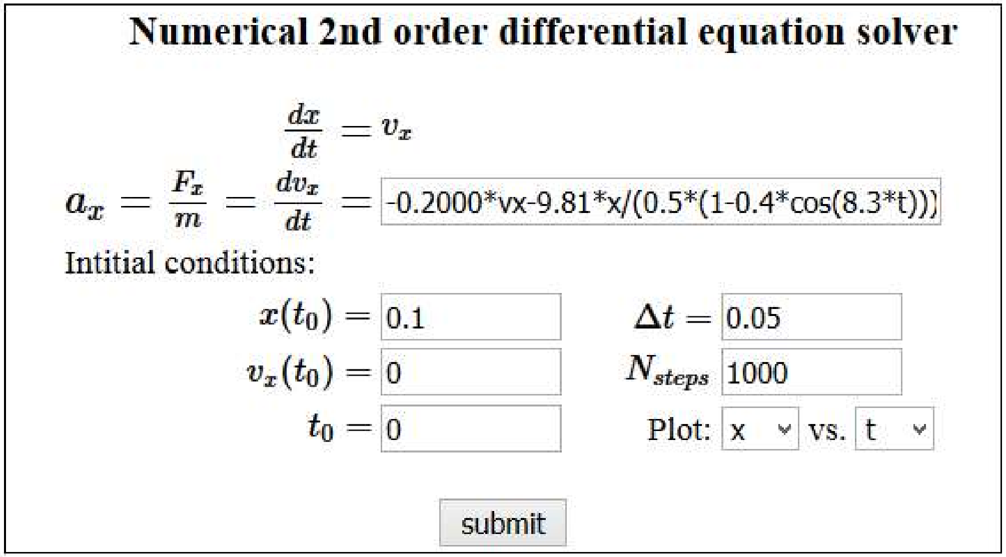
The solutions to a linear differential equation with periodic coefficients,

$$a\frac{d^2y}{dx^2}+b\frac{dy}{dx}+c(x)y=d,$$

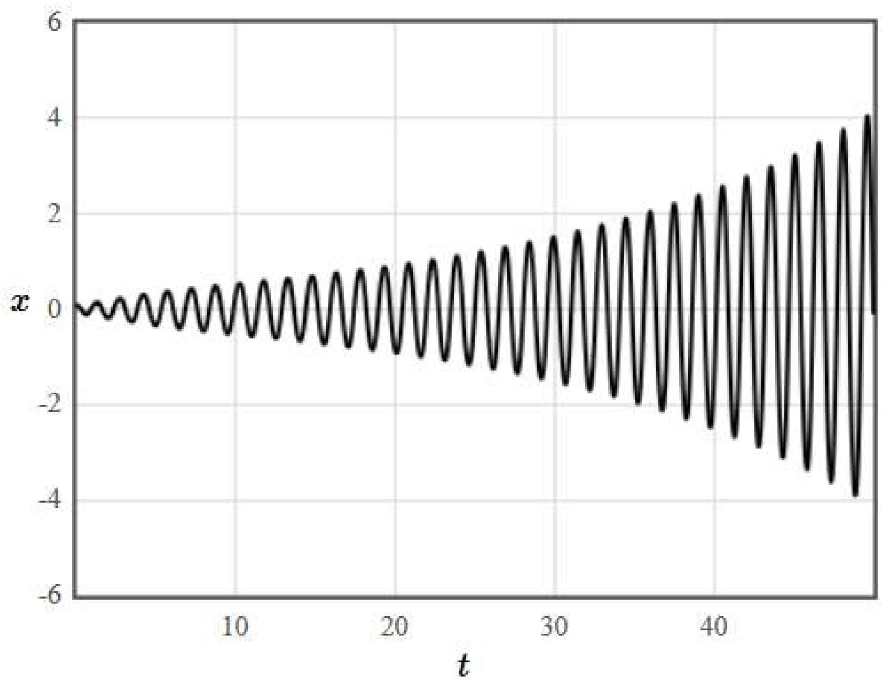
have the form,

$$e^{ikx}u_k(x) \qquad \text{where} \qquad u_k(x)=u_k(x+a)$$

Swing



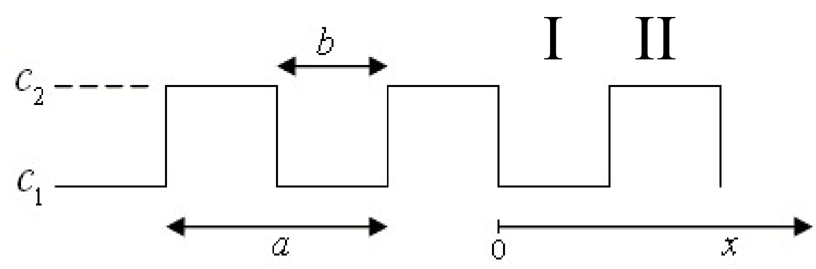
$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + \frac{mg}{l(1 - A\cos(\omega t))}x = 0.$$



For some parameters there are periodic solutions (band).

For some parameters there are exponentially growing and decaying solutions (bandgap).

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.

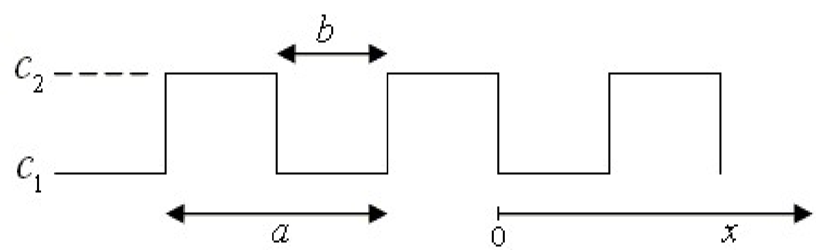
Translational symmetry

The normal modes are eigenfunctions of the translation operator

The normal modes have Bloch form.

$$\xi(x) = e^{ikx} u_k(x) \qquad \text{where} \qquad u_k(x) = u_k(x+a)$$

$$T e^{ikx} u_k(x) = e^{ik(x+a)} u_k(x+a) = e^{ika} e^{ikx} u_k(x)$$



Solutions in region I and region II

Two linearly independent solutions are specified by the boundary conditions

$$\xi_1(0)=1,\quad \xi_1'(0)=0,\quad \xi_2(0)=0,\quad \xi_2'(0)=1$$

In region I,

$$\xi_1(x)=\cos\left(\frac{\omega x}{c_1}\right),\qquad\qquad \xi_2(x)=\frac{c_1}{\omega}\sin\left(\frac{\omega x}{c_1}\right)$$

In region II,

$$\xi_1(x)=\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(x-b)\right)-\frac{c_2}{c_1}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(x-b)\right),$$

$$\xi_2(x)=\frac{c_1}{\omega}\sin\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(x-b)\right)+\frac{c_2}{\omega}\cos\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(x-b)\right)$$

Translation operator

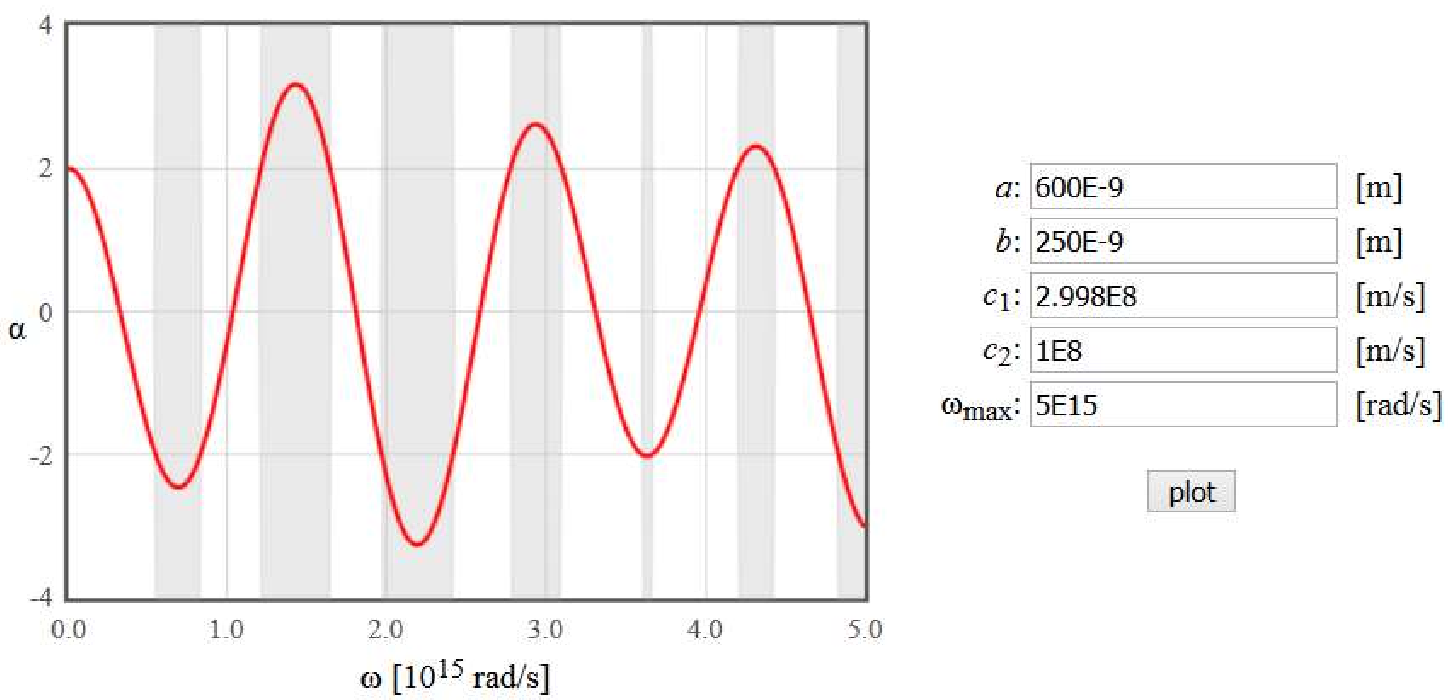
$$\begin{bmatrix} \xi_1(x+a) \\ \xi_2(x+a) \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} \xi_1(x) \\ \xi_2(x) \end{bmatrix}.$$

The elements of the translation matrix can be determined by evaluating this equation and its derivative at $x = 0$. Diagonalize the translation operator and find its eigenvalues to determine the character of the solutions.

Wave vector

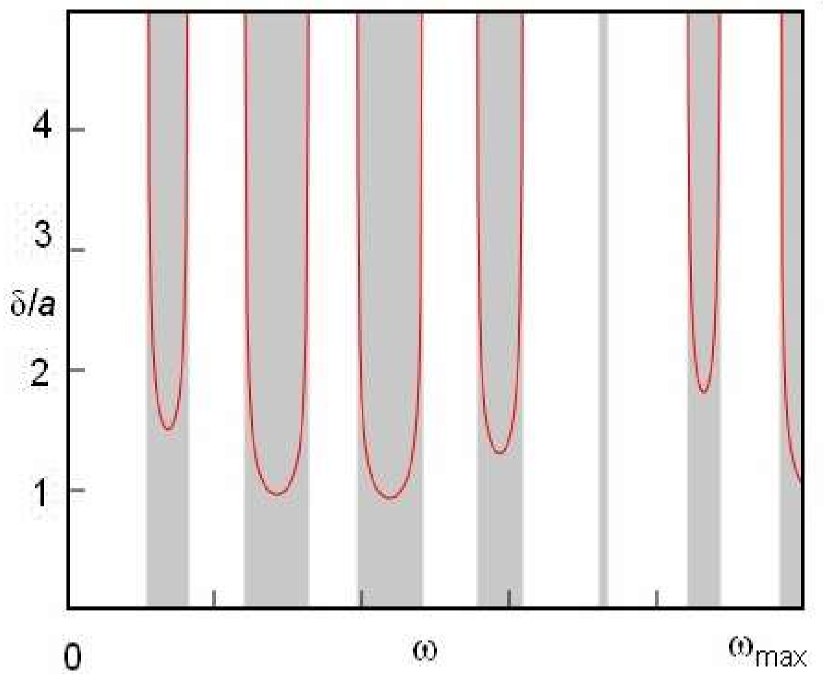
$$k = \frac{1}{a}\tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2} - 1}\right)$$

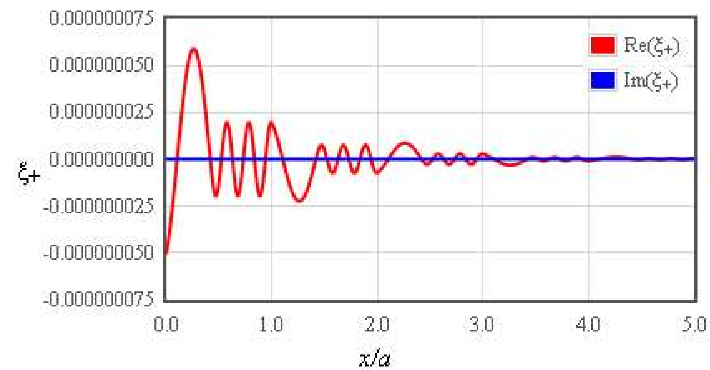
$$\alpha(\omega) = 2\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(a-b)\right) - \frac{c_1^2 + c_2^2}{c_1 c_2}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(a-b)\right)$$

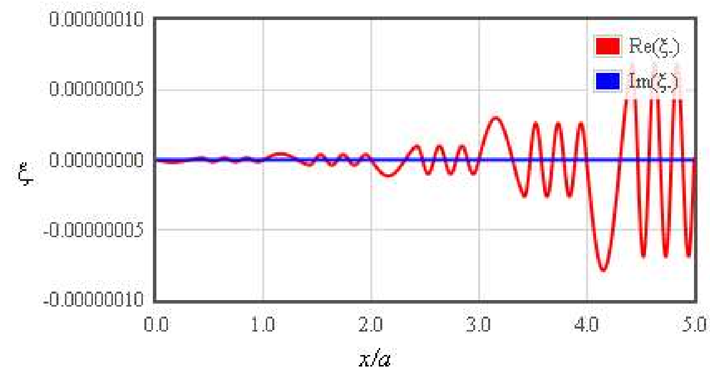


Band gap: exponentially decaying solutions

The one solution grows exponentially and the other decays like exp(-x/δ).



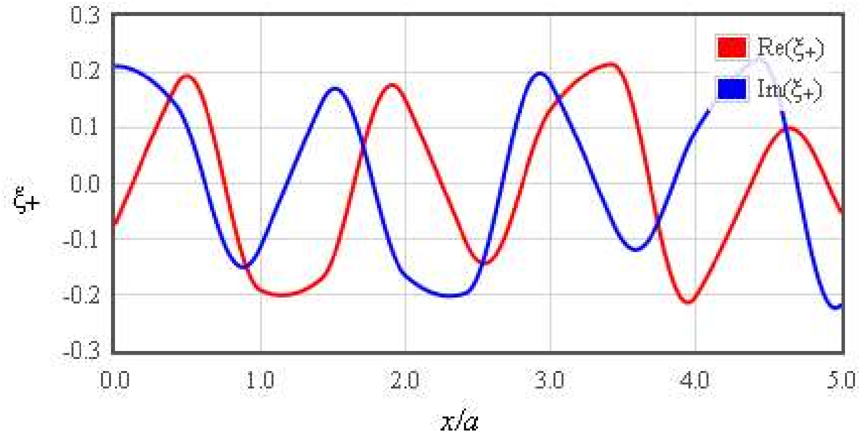




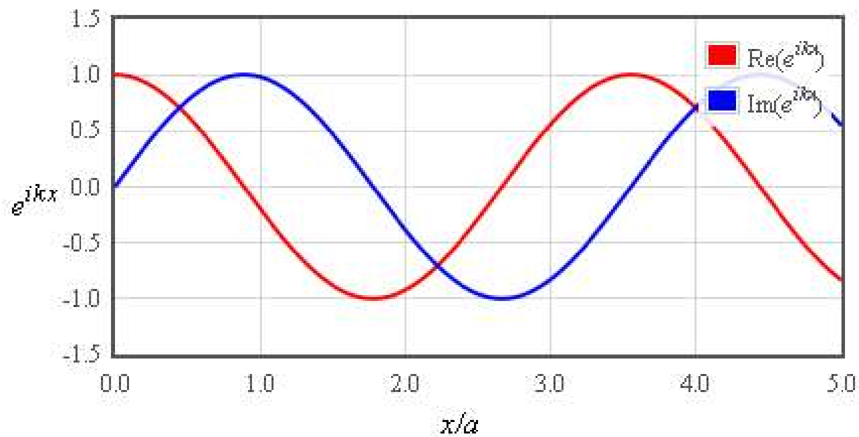
Gray where |α| > 2.

$$\delta = \frac{-a}{\ln\left(\min\left(\lambda_-, \lambda_+\right)\right)}$$

Bloch waves

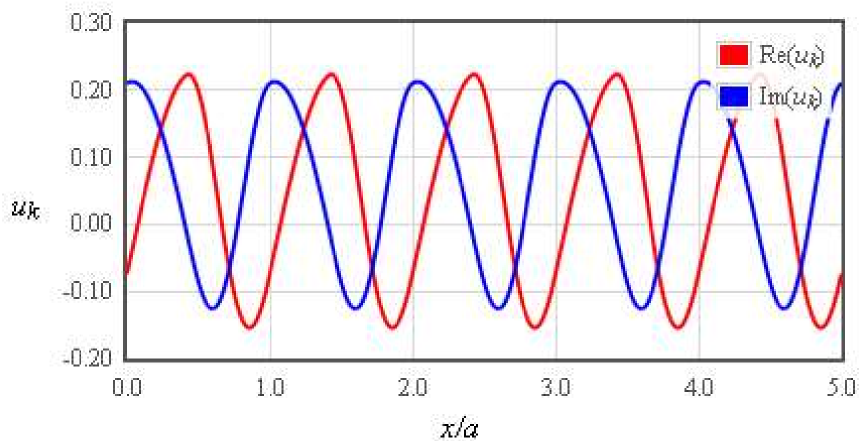


$$\xi = e^{ikx} u_k(x)$$



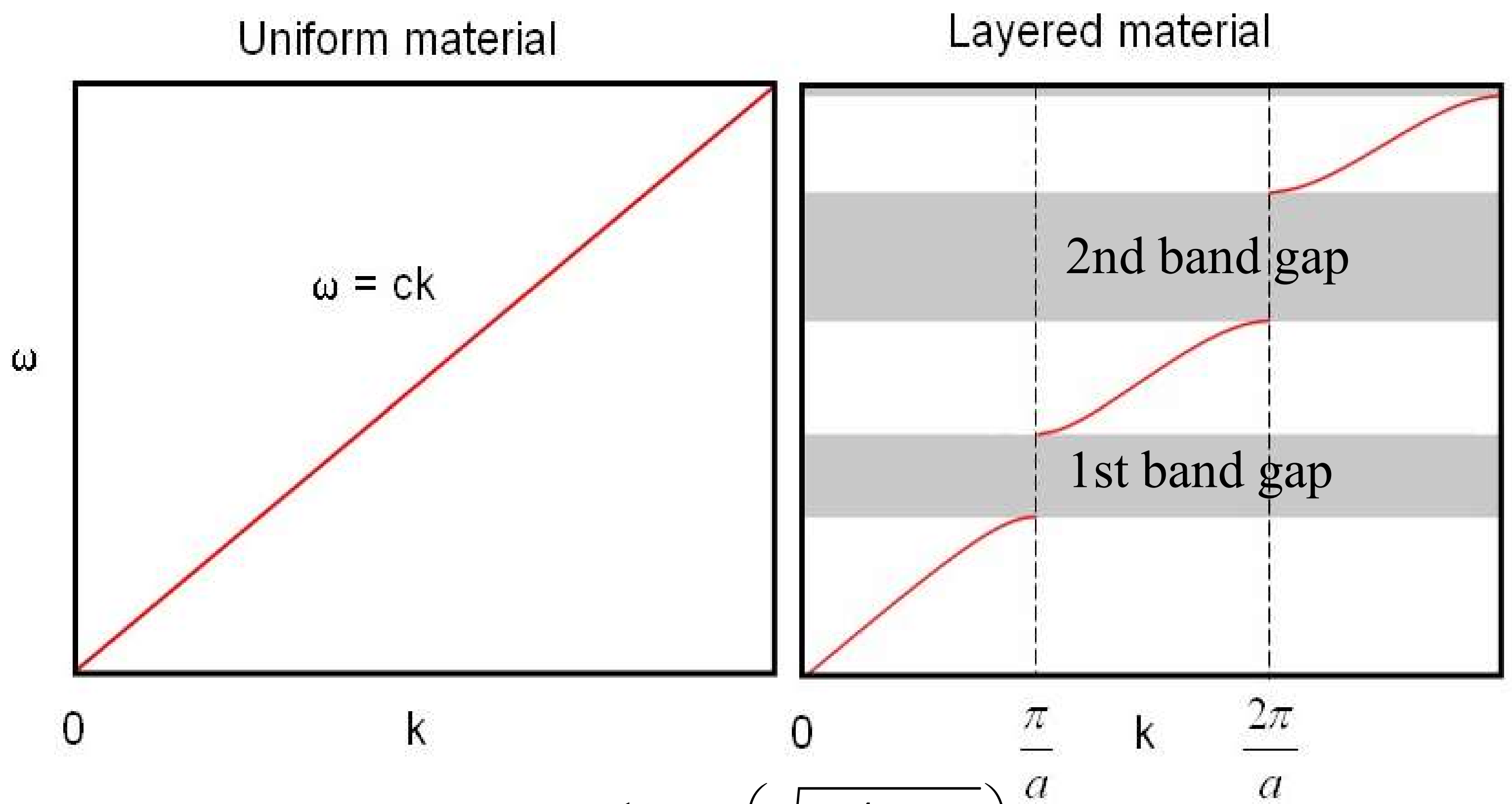
For periodic boundary conditions $L = Na$, the allowed values of k are exactly those allowed for waves in vacuum.

k labels the eigenfunctions of the translation operator.



$$Te^{ikx} u_k(x) = e^{ik(x+a)} u_k(x+a) = e^{ika} e^{ikx} u_k(x)$$

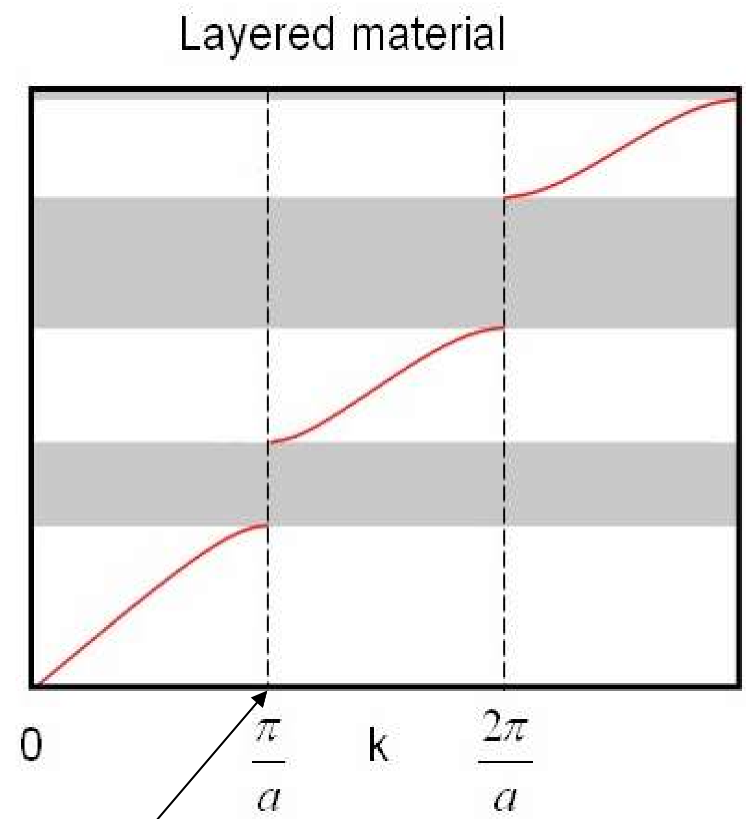
Dispersion relation

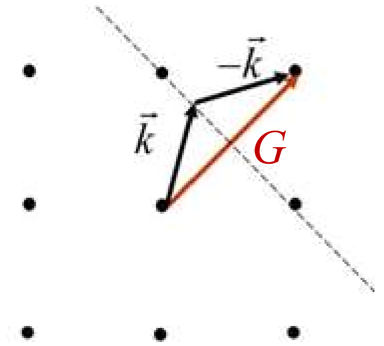


$$k = \frac{1}{a} \tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2} - 1} \right)$$

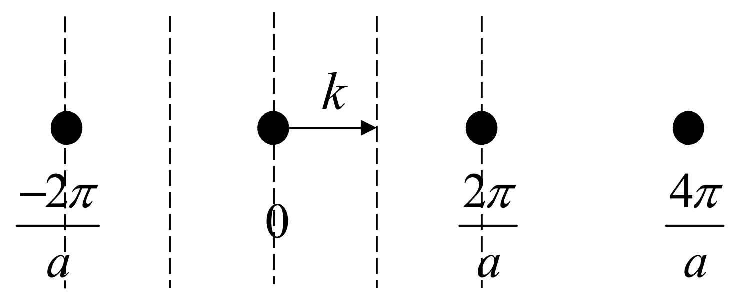
$$\alpha(\omega) = 2\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(a-b)\right) - \frac{c_1^2 + c_2^2}{c_1 c_2}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(a-b)\right)$$

Diffraction condition



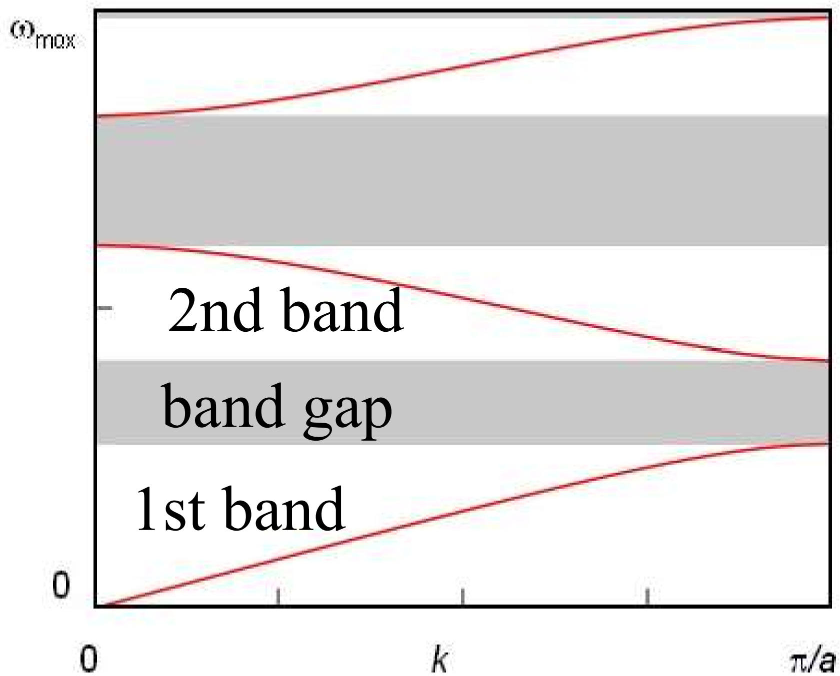


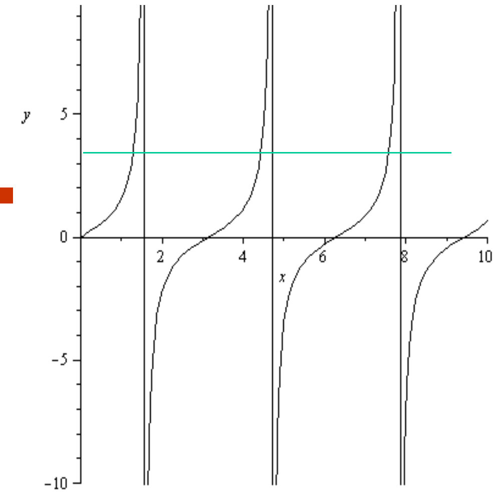
1st Brilluoin zone boundary



Dispersion relation

$$k = \frac{1}{a}\tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2} - 1}\right)$$





$$\tan(ka) = \sqrt{\frac{4}{\alpha^2} - 1}$$

$$e^{ikx}u_k(x) = e^{ikx}\sum_G a_G e^{iGx}$$

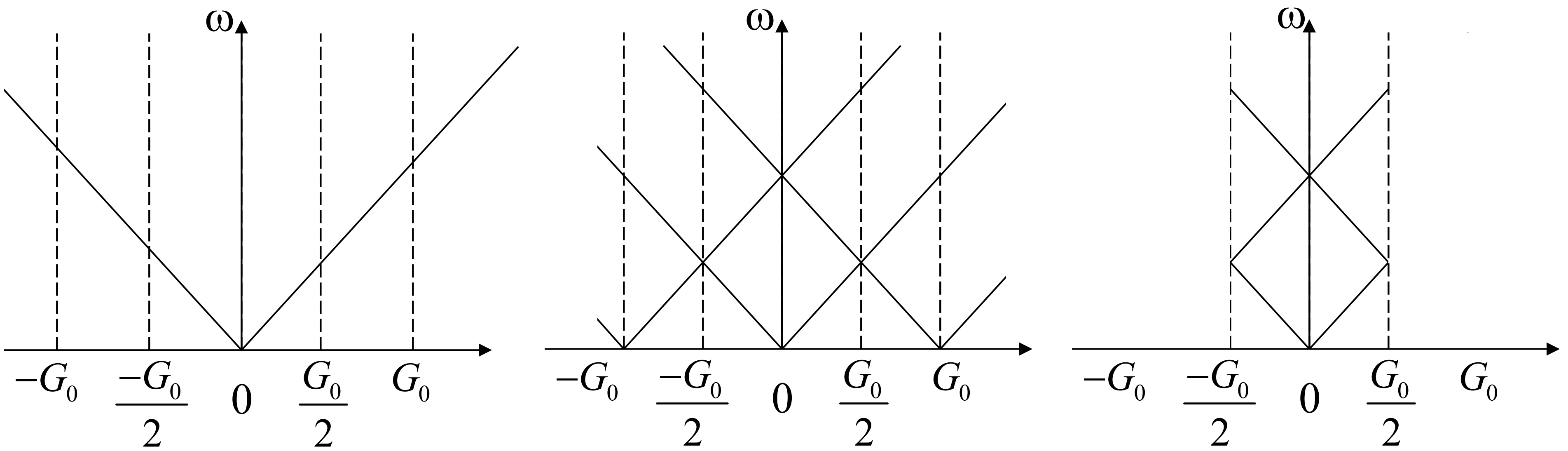
$$k = k' + G'$$

$$e^{ikx}u_k(x) = e^{i(k'+G')x}\sum_G a_G e^{iGx}$$

$$e^{ikx}u_k(x) = e^{ik'x}\sum_G a_G e^{i(G+G')x}$$

There is only one *k*' in the first Brillouin zone and the convention is to use that one.

Zone schemes

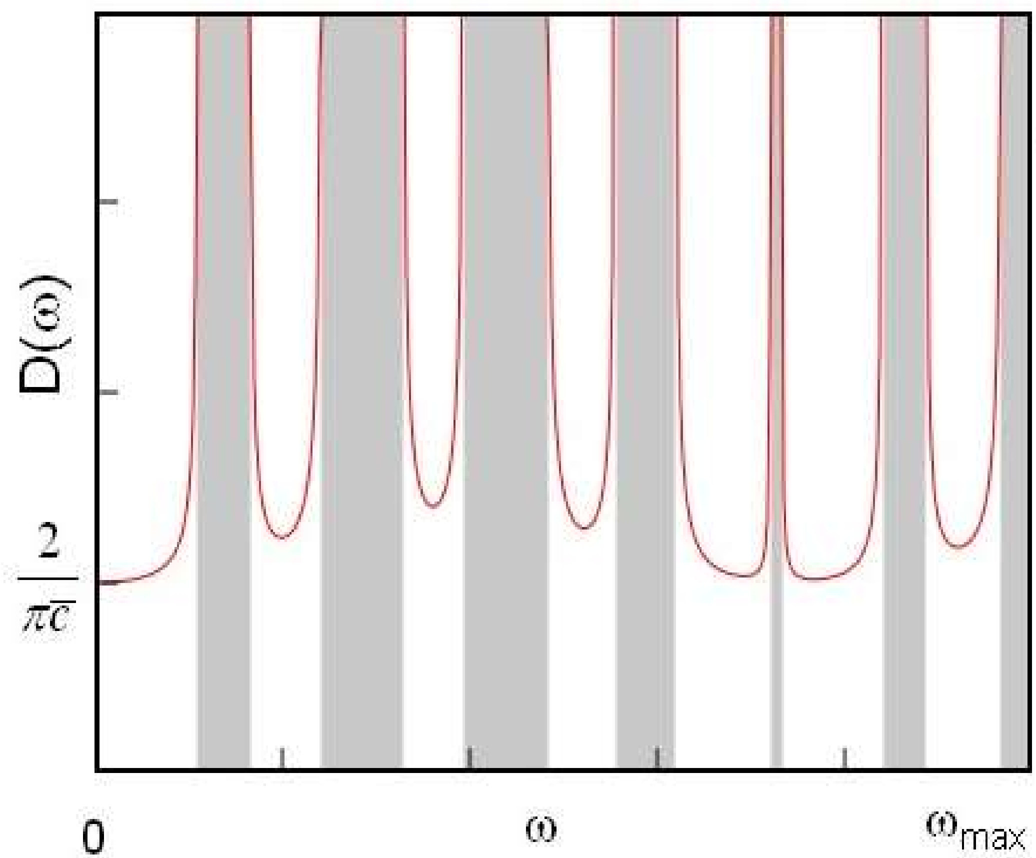


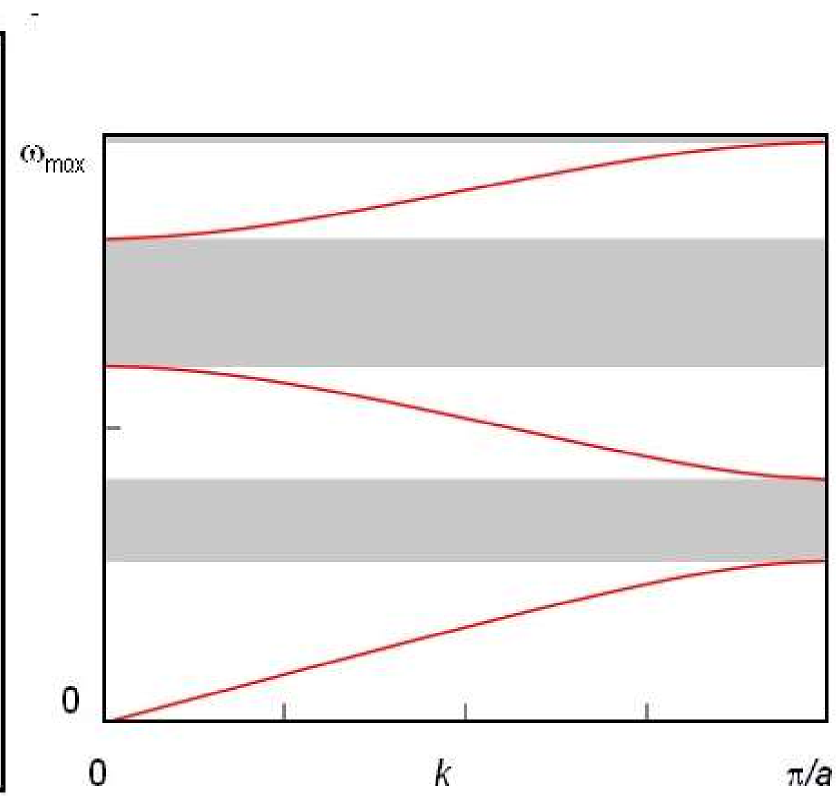
Extended

Repeated

Reduced

Density of states

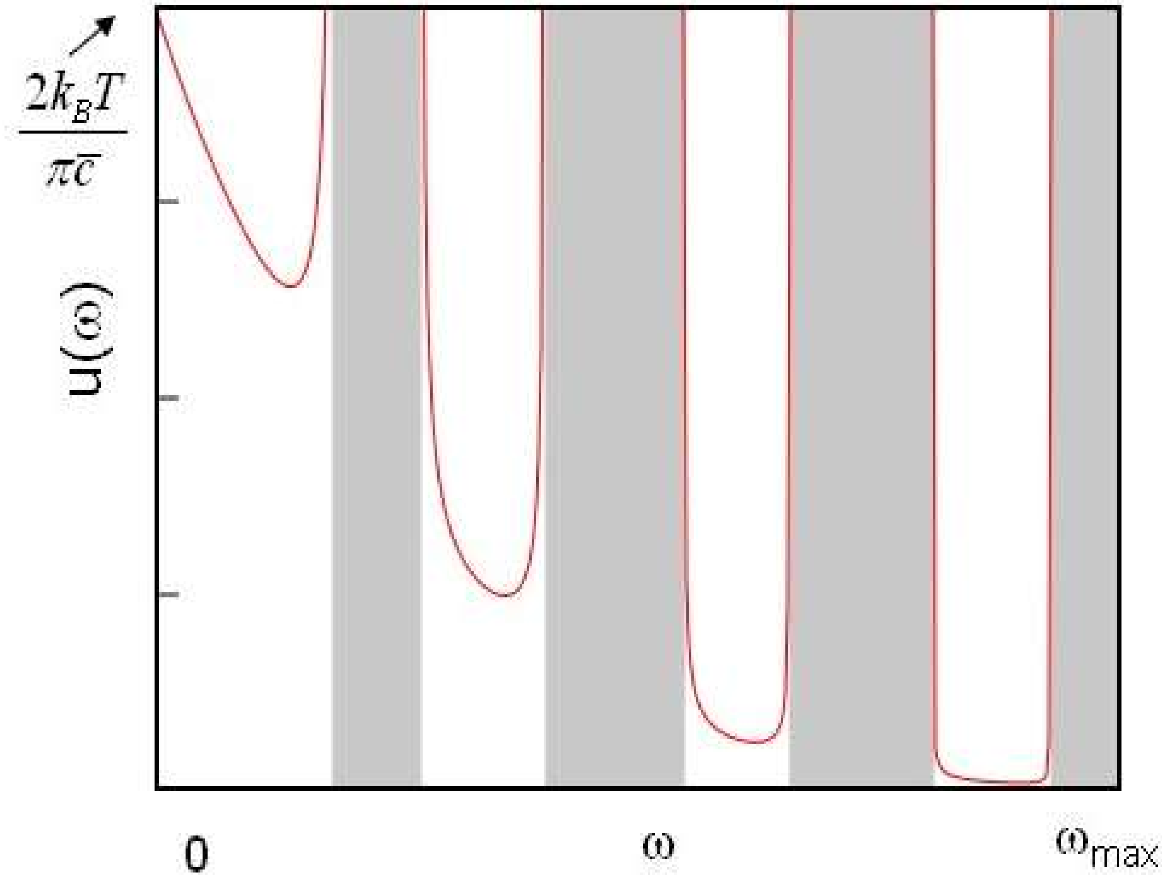




$$D(\omega) = D(k)\frac{dk}{d\omega}$$

The density of states can be determined from the dispersion relation.

Energy spectral density



$$u(\omega) = \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

Analog to the Planck radiation curve.

Thermodynamic quantities

Energy spectral density: $$u(\omega) = \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$ DoS → u(ω)

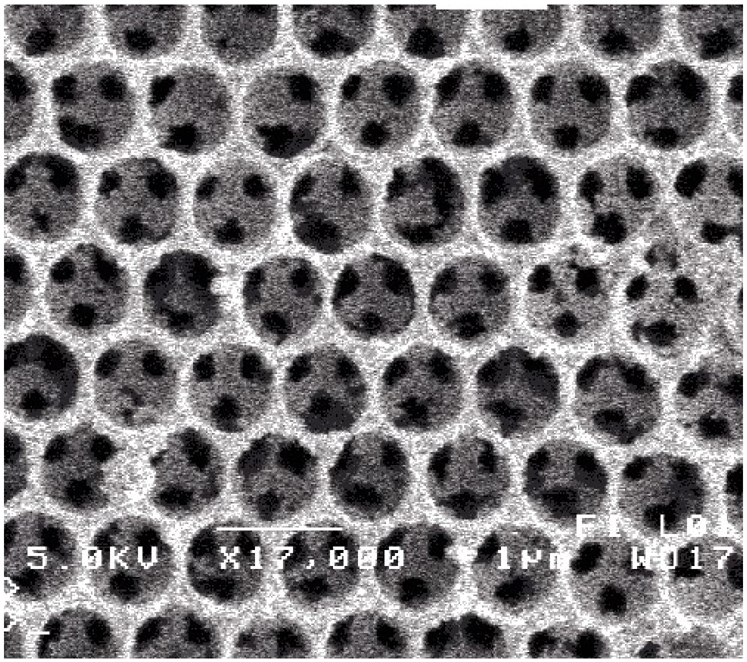
Internal energy density: $$u(T) = \int_0^\infty \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega$$ DoS → u(T)

Helmholz free energy density: $$f(T) = k_B T \int_0^\infty D(\omega) \ln\left(1 - \exp\left(\frac{-\hbar\omega}{k_B T}\right)\right) d\omega$$ DoS → f(T)

Entropy density: $$s = -\frac{\partial f}{\partial T} = -k_B \int_0^\infty D(\omega) \left(\ln\left(1 - e^{-\hbar\omega/k_B T}\right) + \frac{\hbar\omega}{k_B T\left(1 - e^{\hbar\omega/k_B T}\right)} \right) d\omega$$ DoS → s(T)

Specific heat: $$c_v = \int \left(\frac{\hbar\omega}{T}\right)^2 \frac{D(\omega)\exp\left(\frac{\hbar\omega}{k_B T}\right)}{k_B\left(\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1\right)^2} d\omega$$ DoS → cv(T)

Inverse opal photonic crystal



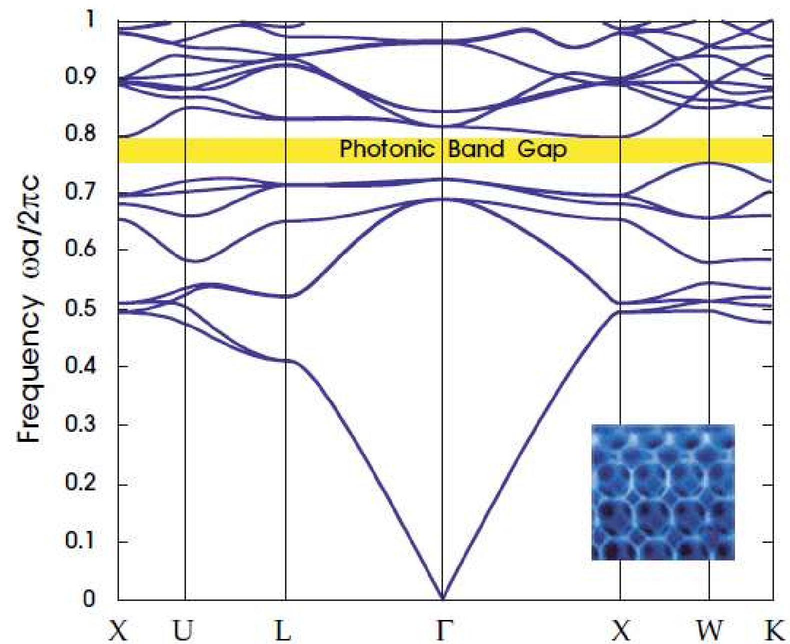
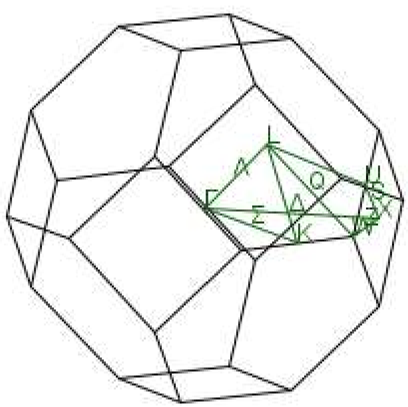


Figure 8: The photonic band structure for the lowest bands of an "inverse opal" structure: a face-centered cubic (fcc) lattice of close-packed air spheres in dielectric ($\varepsilon = 13$). (Inset shows fabricated structure from figure 9.) There is a complete photonic band gap (yellow) between the eighth 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.



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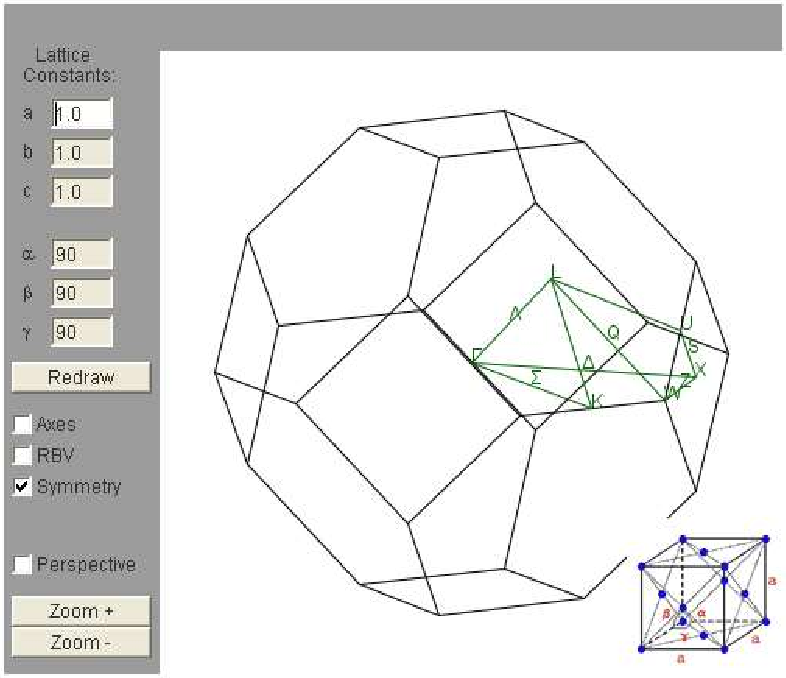
The first Brillouin zone of a face centered cubic lattice



$$\vec{k} = u\vec{b}_1 + v\vec{b}_2 + w\vec{b}_3 \quad : \quad (u,v,w)$$

Symmetry points (u,v,w)	[kx,ky,kz]	Point group
Γ: (0,0,0)	[0,0,0]	m3m
X: (0,1/2,1/2)	[0,2π/a,0]	4/mmm
L: (1/2,1/2,1/2)	[π/a,π/a,π/a]	$\bar{3}$m
W: (1/4,3/4,1/2)	[π/a,2π/a,0]	$\bar{4}$2m
U: (1/4,5/8,5/8)	[π/2a,2π/a,π/2a]	mm2
K: (3/8,3/4,3/8)	[3π/2a,3π/2a,0]	mm2

$$\overline{\Gamma L} = \frac{\sqrt{3}\pi}{a}, \quad \overline{\Gamma X} = \frac{2\pi}{a}, \quad \overline{\Gamma W} = \frac{\sqrt{5}\pi}{a}$$

$$\overline{\Gamma K} = \overline{\Gamma U} = \frac{3\pi}{\sqrt{2}a}, \quad \overline{KW} = \overline{XU} = \frac{\pi}{\sqrt{2}a}$$

Symmetry lines	Point group
Δ: (0,v,v) 0 < v < 1/2	4mm
Λ: (w,w,w) 0 < w < 1/2	3m
Σ: (u,2u,u) 0 < u < 3/8	mm2
S: (2u,1/2+2u,1/2+u) 0 < u < 1/8	mm2
Z: (u,1/2+u,1/2) 0 < u < 1/4	mm2
Q: (1/2-u,1/2+u,1/2) 0 < u < 1/4	2

The real space and reciprocal space primitive translation vectors are:

$$\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{z}), \qquad \vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{y}), \qquad \vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{z}),$$

$$\vec{b}_1 = \frac{2\pi}{a}\left(\hat{k}_x - \hat{k}_y + \hat{k}_z\right), \quad \vec{b}_2 = \frac{2\pi}{a}\left(\hat{k}_x + \hat{k}_y - \hat{k}_z\right), \quad \vec{b}_3 = \frac{2\pi}{a}\left(-\hat{k}_x + \hat{k}_y + \hat{k}_z\right)$$

Cut-out patterns for Brillouin zones

Cut-out patterns to make your own models of the Brillouin zones. The symmetry points are red and the symmetry lines are blue.

- simple cubic
- face centered cubic
- body centered cubic
- hexagonal
- tetragonal
- body centered tetragonal
- orthorhombic
- face centered orthorhombic
- body centered orthorhombic
- base centered orthorhombic