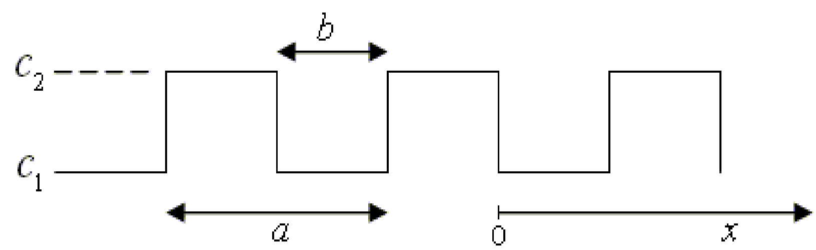
Technische Universität Graz

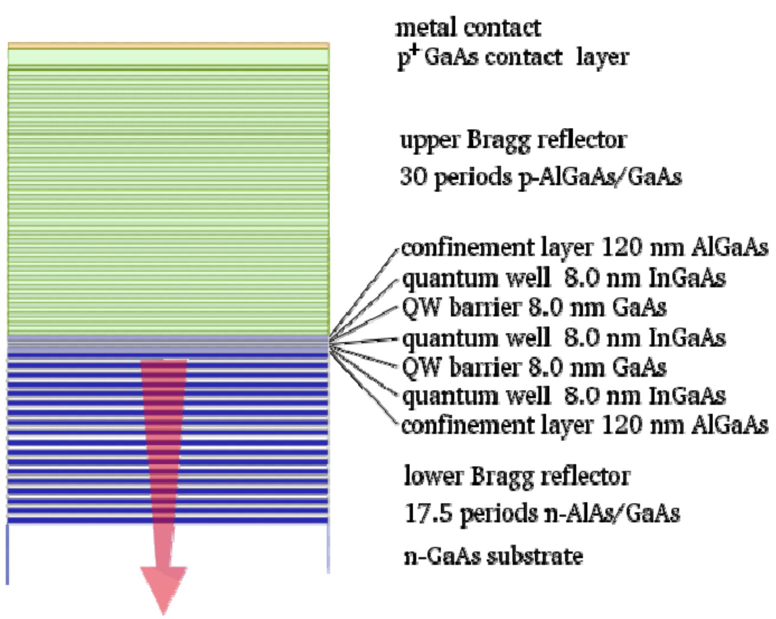
13. Photons

May 3, 2018

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,

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

Swing

Numerical 2nd order differential equation solver

$$\frac{dx}{dt} = v_x$$

$$a_x = \frac{F_x}{m} = \frac{dv_x}{dt} = \text{-0.2000*vx-9.81*x/(0.5*(1-0.4*cos(8.3*t)))}$$

Intitial conditions:

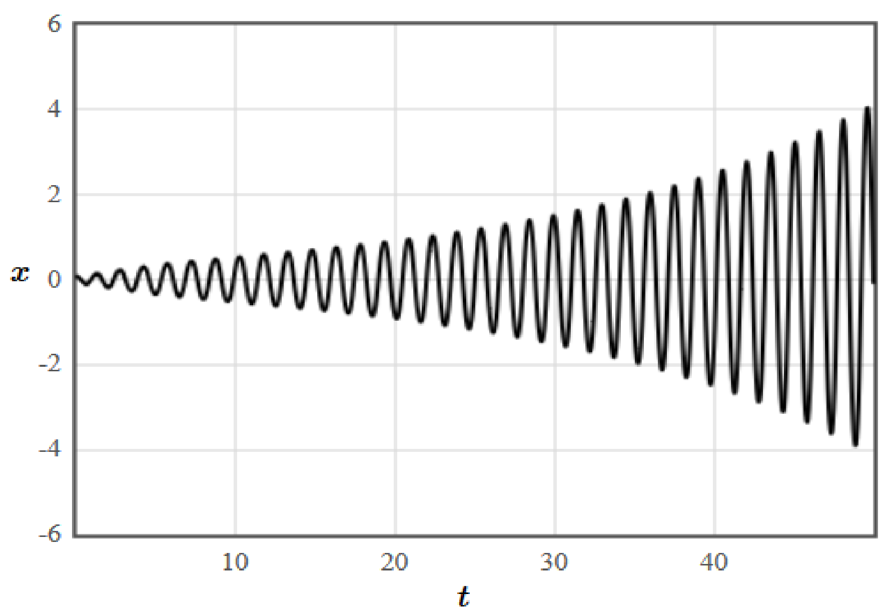
$x(t_0) =$ 0.1 $\quad \Delta t =$ 0.05

$v_x(t_0) =$ 0 $\quad N_{steps}$ 1000

$t_0 =$ 0 $\quad$ Plot: x vs. t

submit

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



For some parameters there are periodic solutions (band).

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

http://lampx.tugraz.at/~hadley/physikm/apps/numerical_integration/parametric.de.php

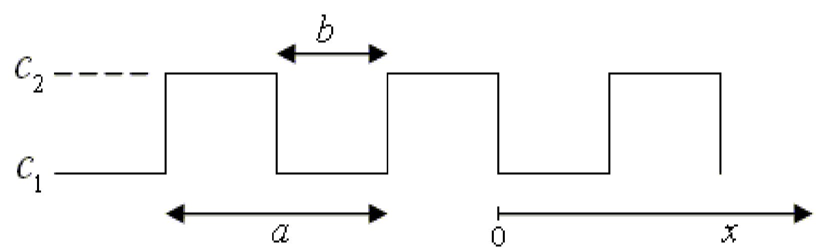
Translational symmetry

The normal modes are eigenfunctions of the translation operator

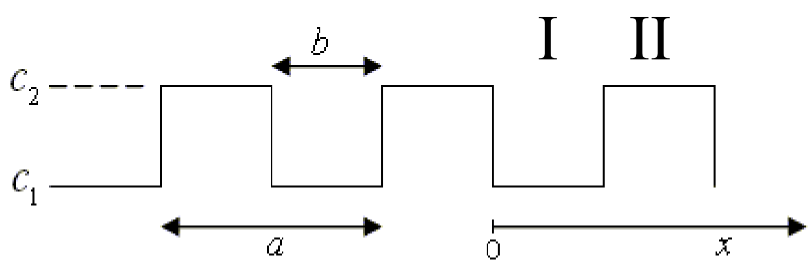
The normal modes have Bloch form.

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

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



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.

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,

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

In region II,

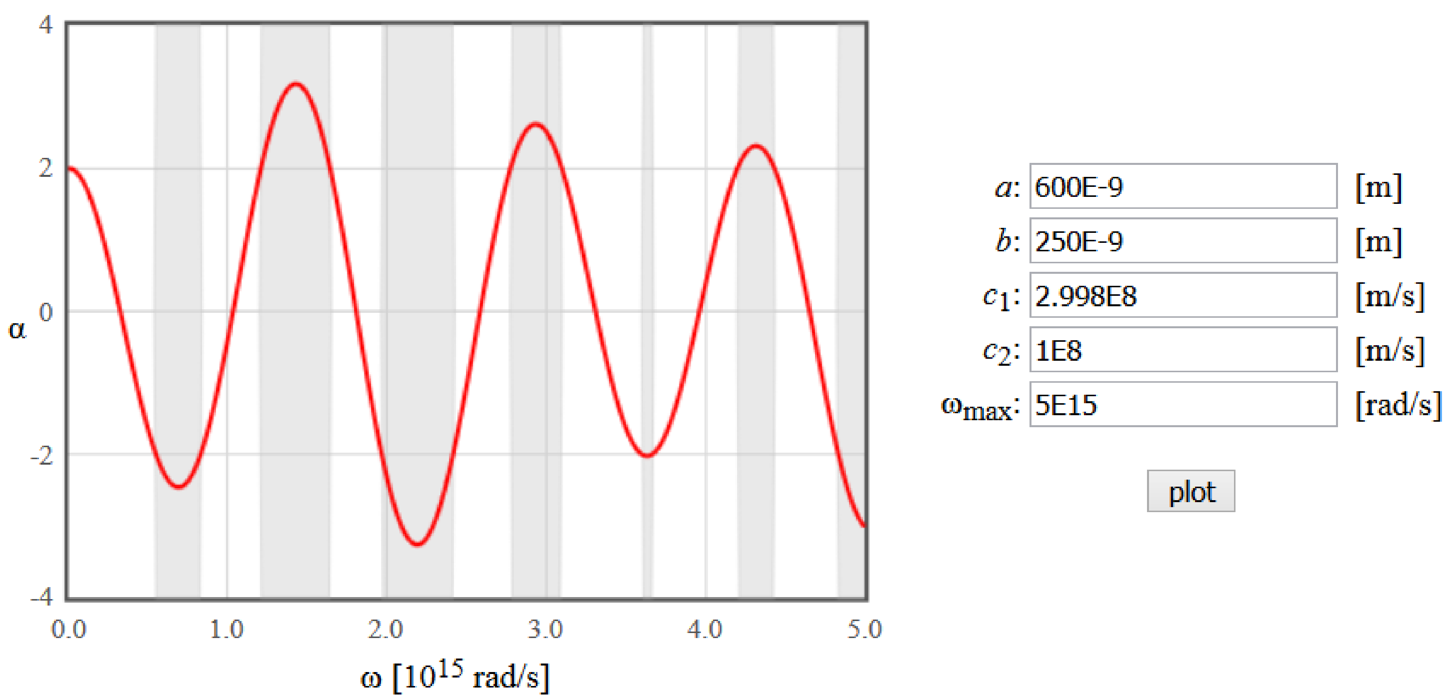
$$\xi_1(x)=\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(x-b)\right)-\frac{c_2}{c_1}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(x-b)\right),$$

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

Wave vector

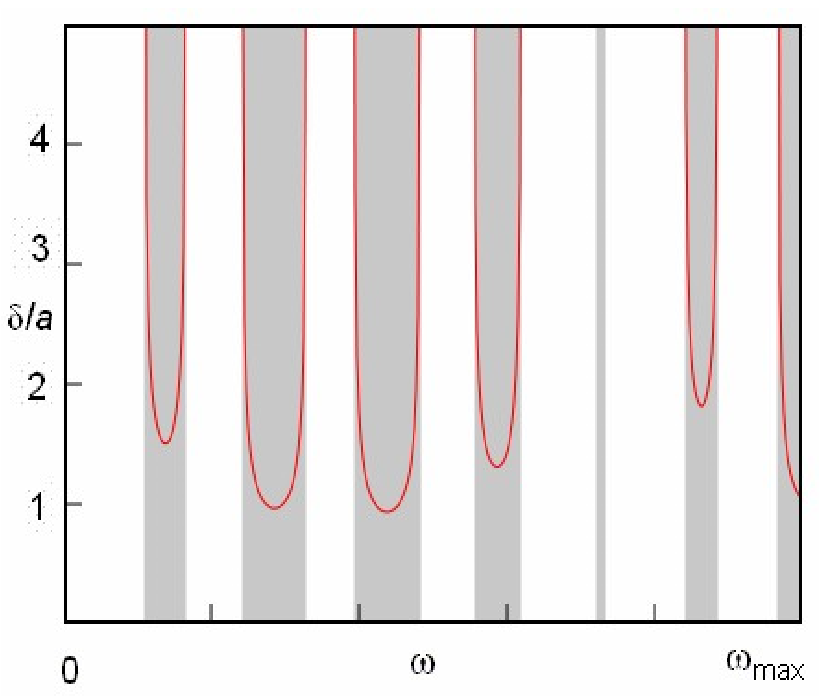
$$k = \frac{1}{a}\tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2} - 1}\right)$$

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

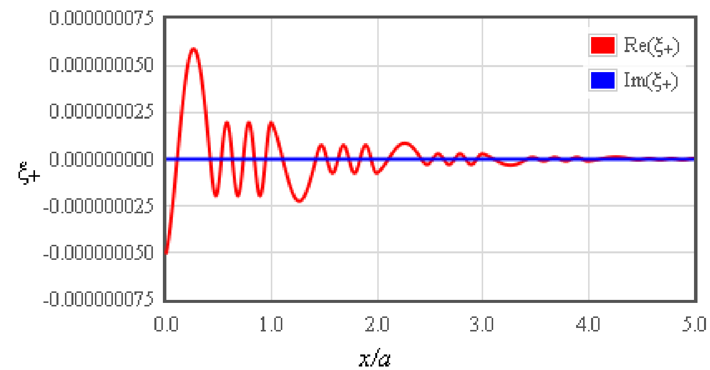


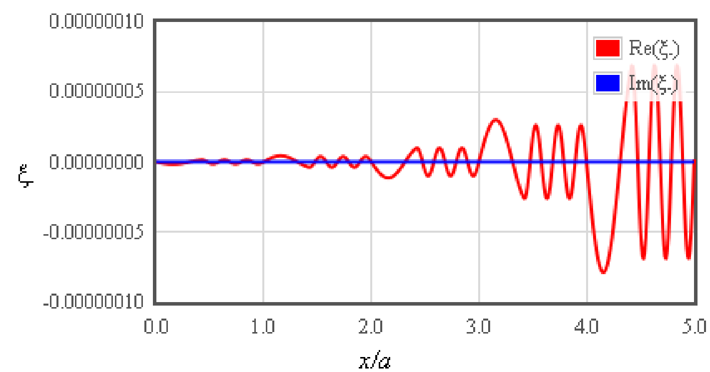
Band gap: exponentially growing solutions

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



Gray where |α| > 2.

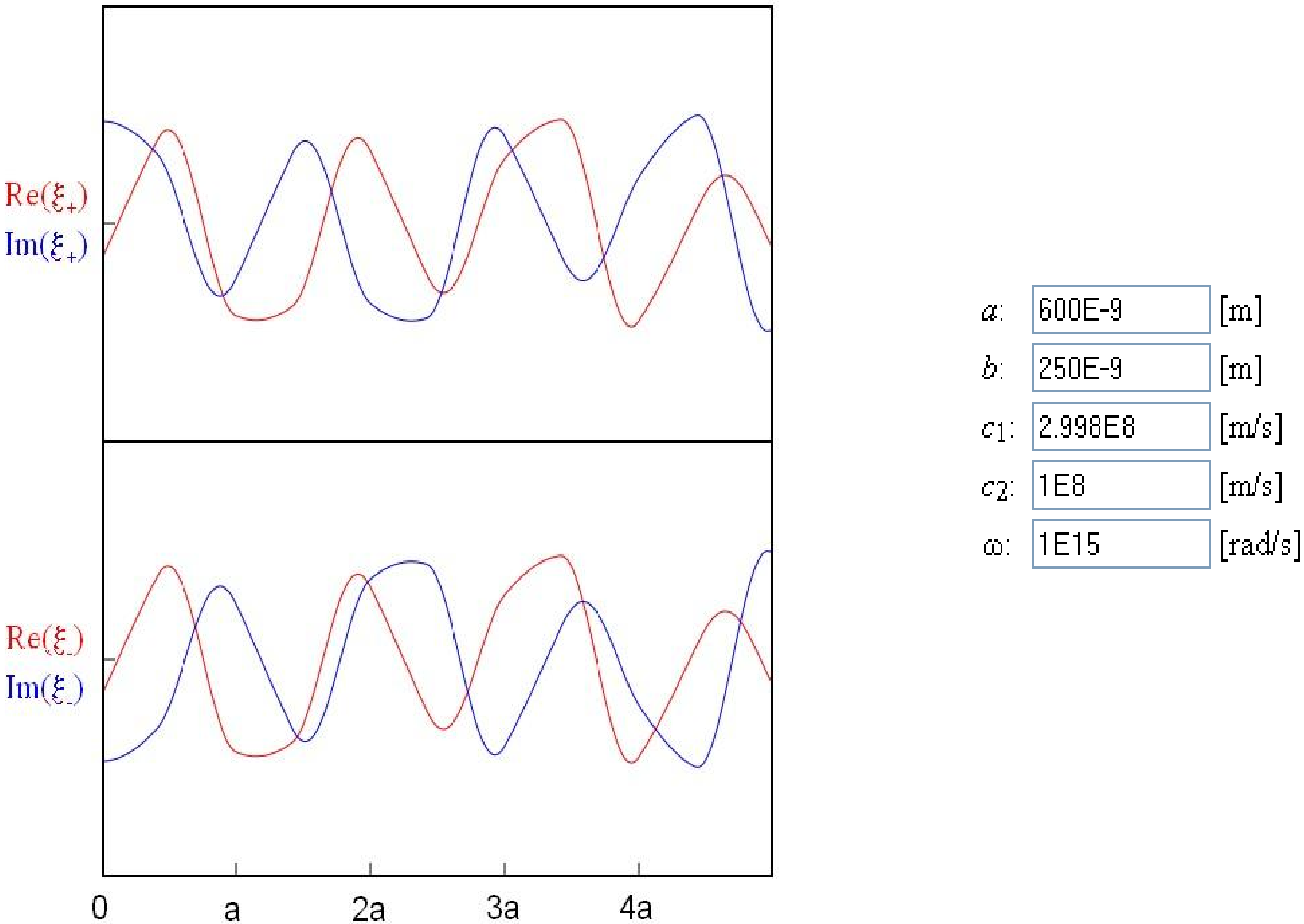


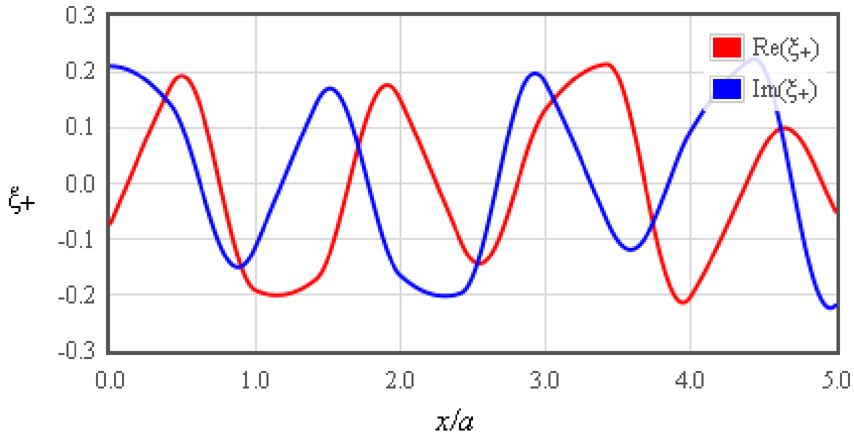


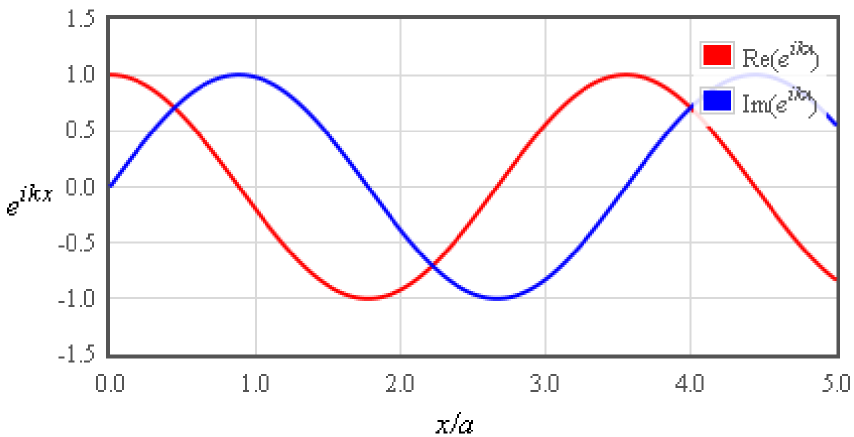
$$\delta = \frac{-a}{\ln\left(\min\left(\lambda_-, \lambda_+\right)\right)}$$

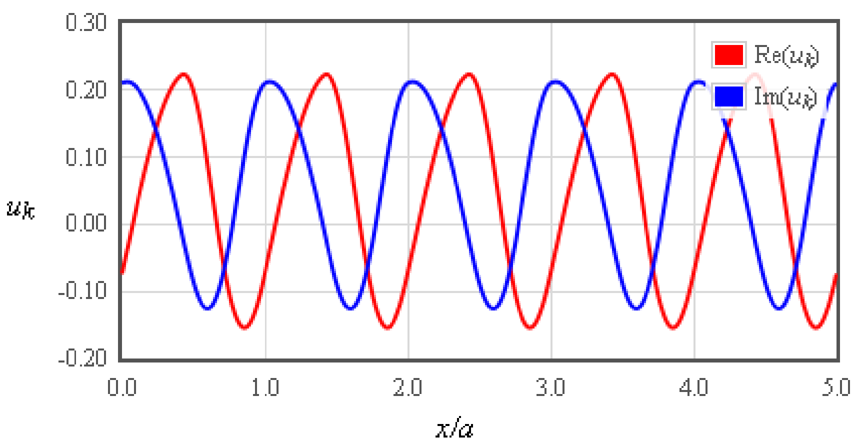
Band: Bloch waves

The solutions have the form $e^{ikx}u_k(x)$ where $u_k(x+a)=u_k(x)$









Bloch waves

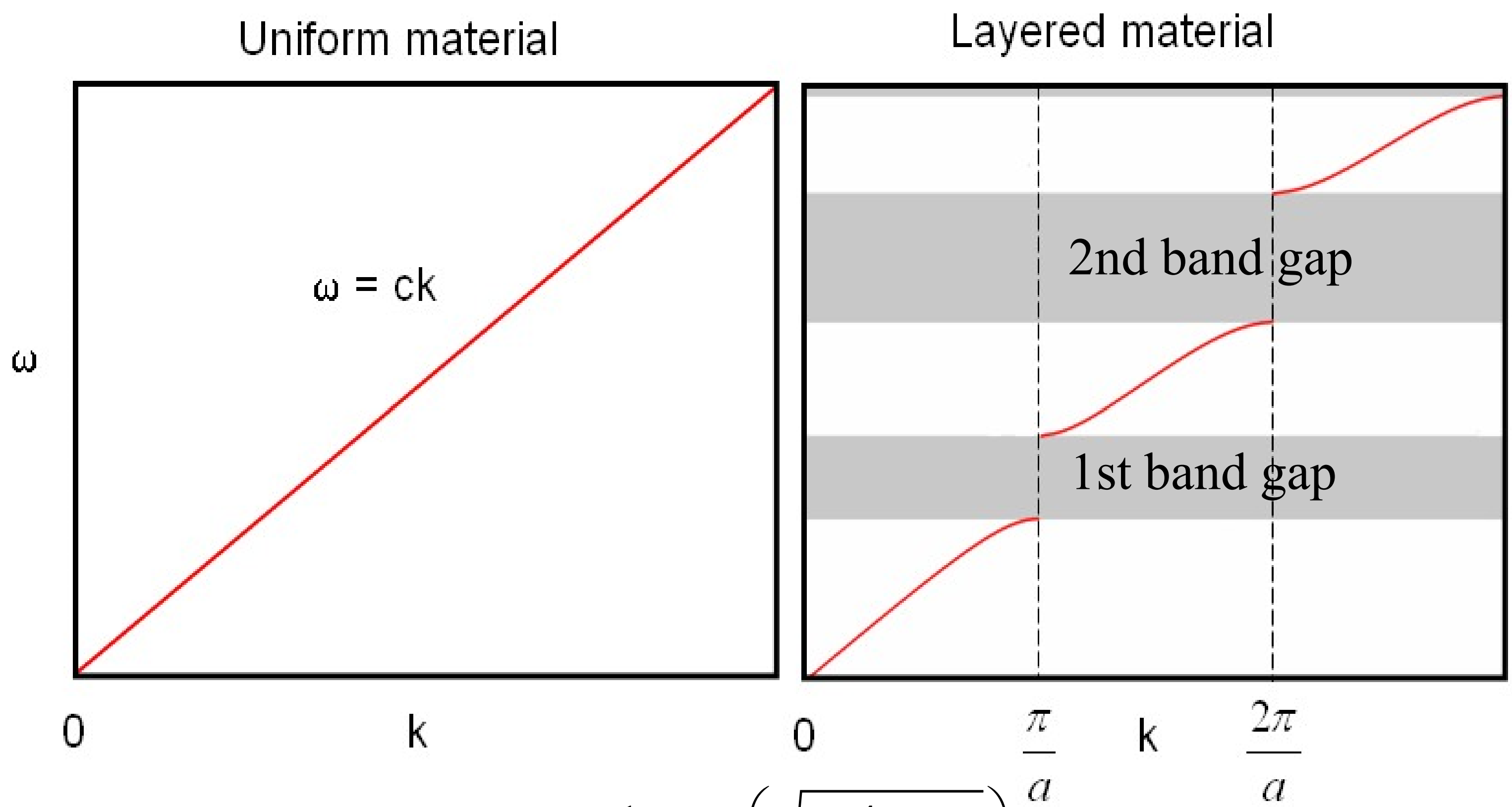
$$\xi = e^{ikx} u_k(x)$$

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.

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

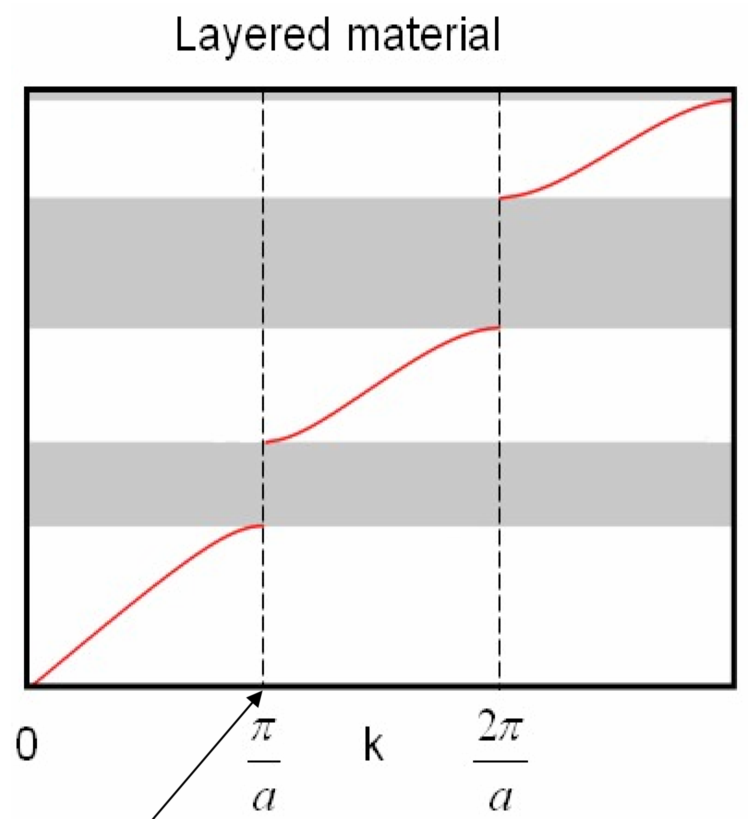
Dispersion relation

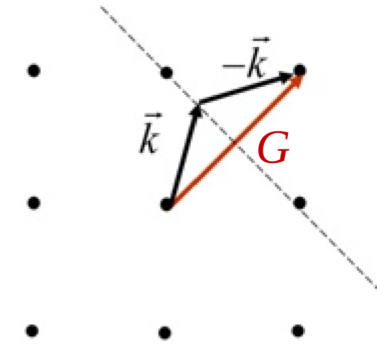


$$k = \frac{1}{a}\tan^{-1}\left(\sqrt{\frac{4}{\alpha(\omega)^2} - 1}\right)$$

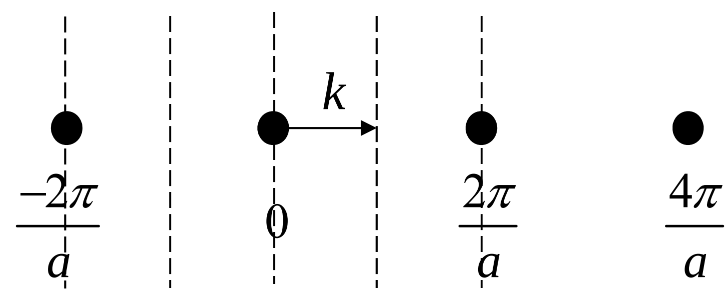
$$\alpha(\omega) = 2\cos\left(\frac{\omega b}{c_1}\right)\cos\left(\frac{\omega}{c_2}(a-b)\right) - \frac{c_1^2 + c_2^2}{c_1 c_2}\sin\left(\frac{\omega b}{c_1}\right)\sin\left(\frac{\omega}{c_2}(a-b)\right)$$

Diffraction condition

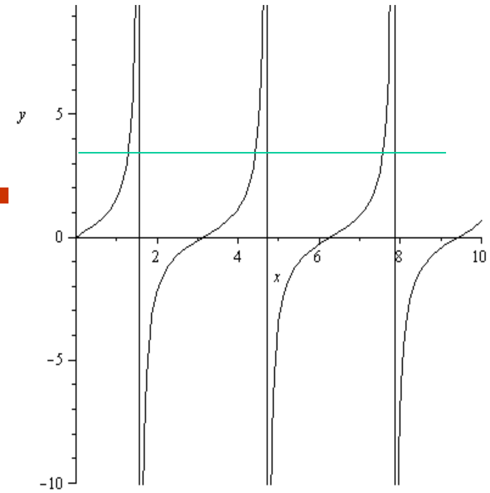




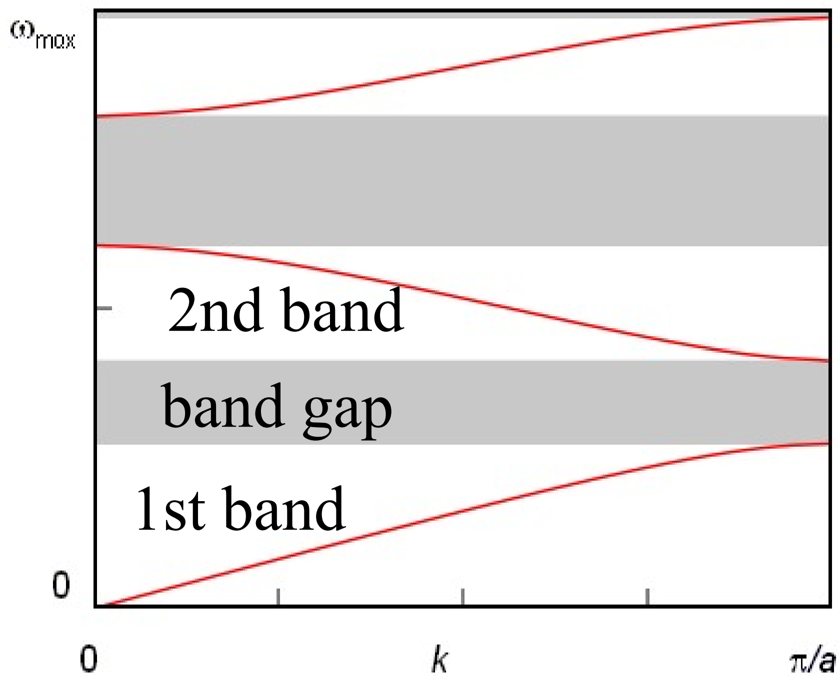
1st Brilluoin zone boundary



Dispersion relation



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



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

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

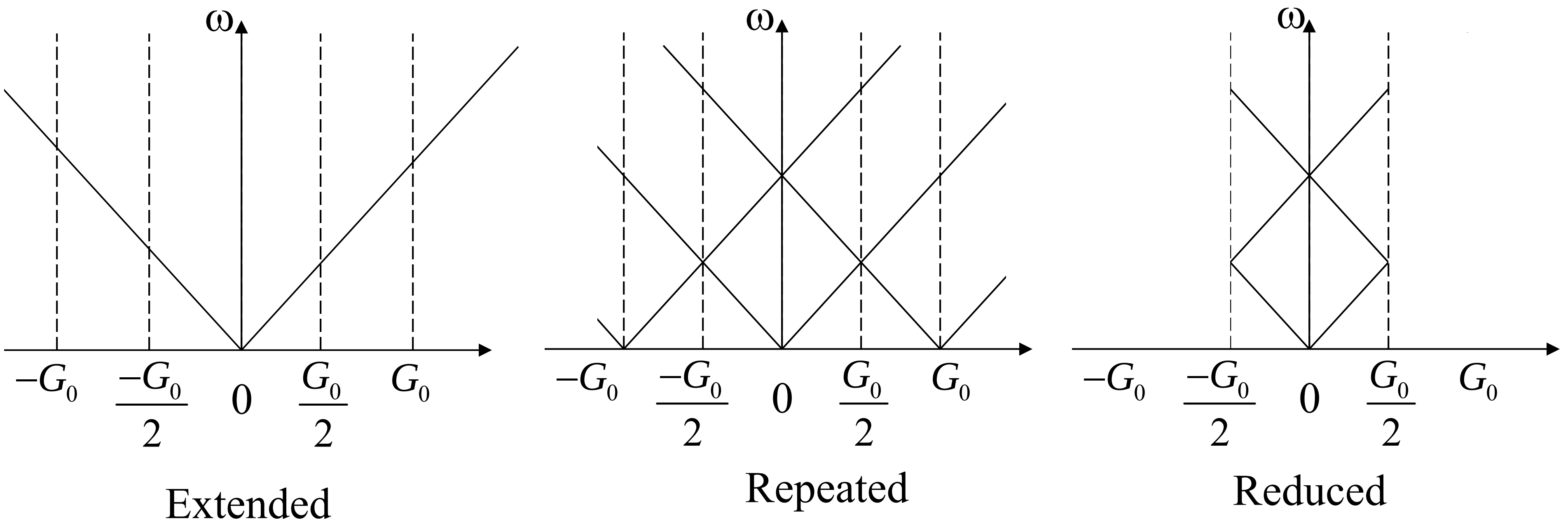
$$k = k' + G'$$

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

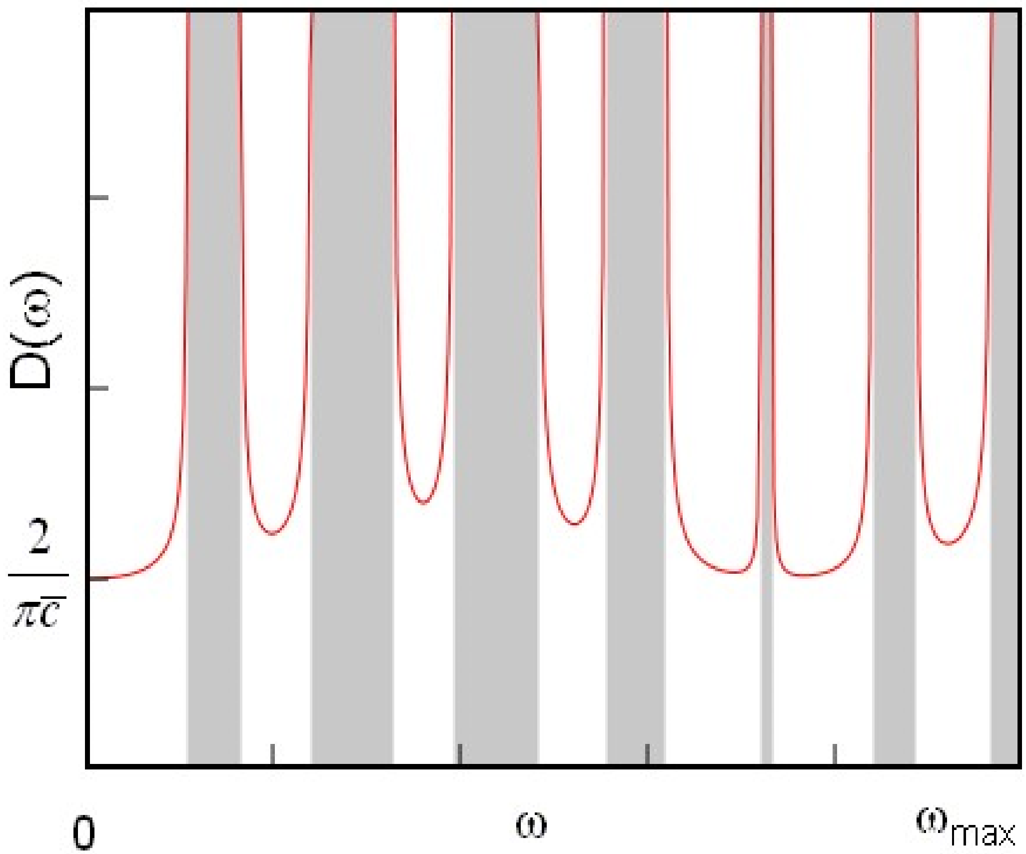
$$e^{ikx}u_k(x) = e^{ik'x}\sum_G a_G e^{i(G+G')x}$$

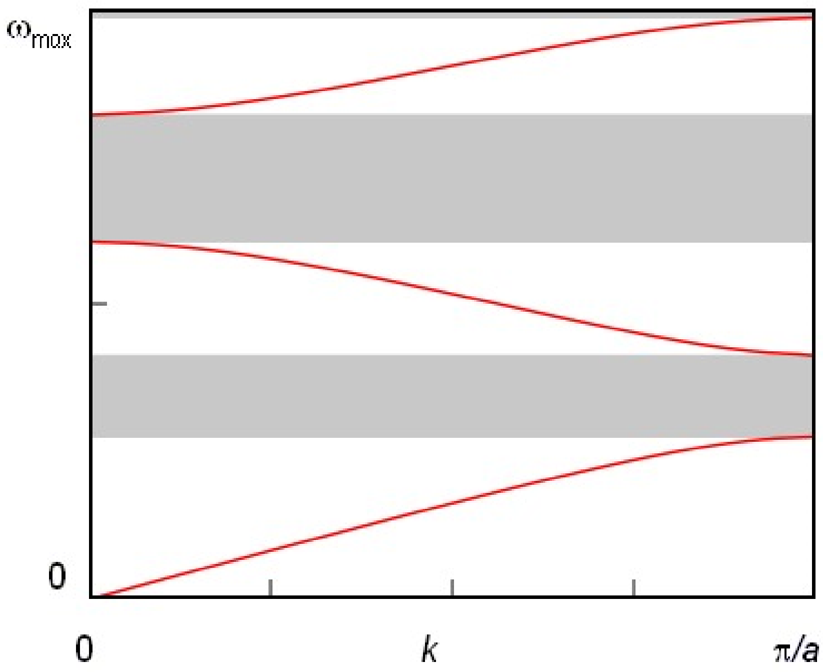
There is only one *k*' in the first Brillouin zone and the convention is to use that one.

Zone schemes



Density of states

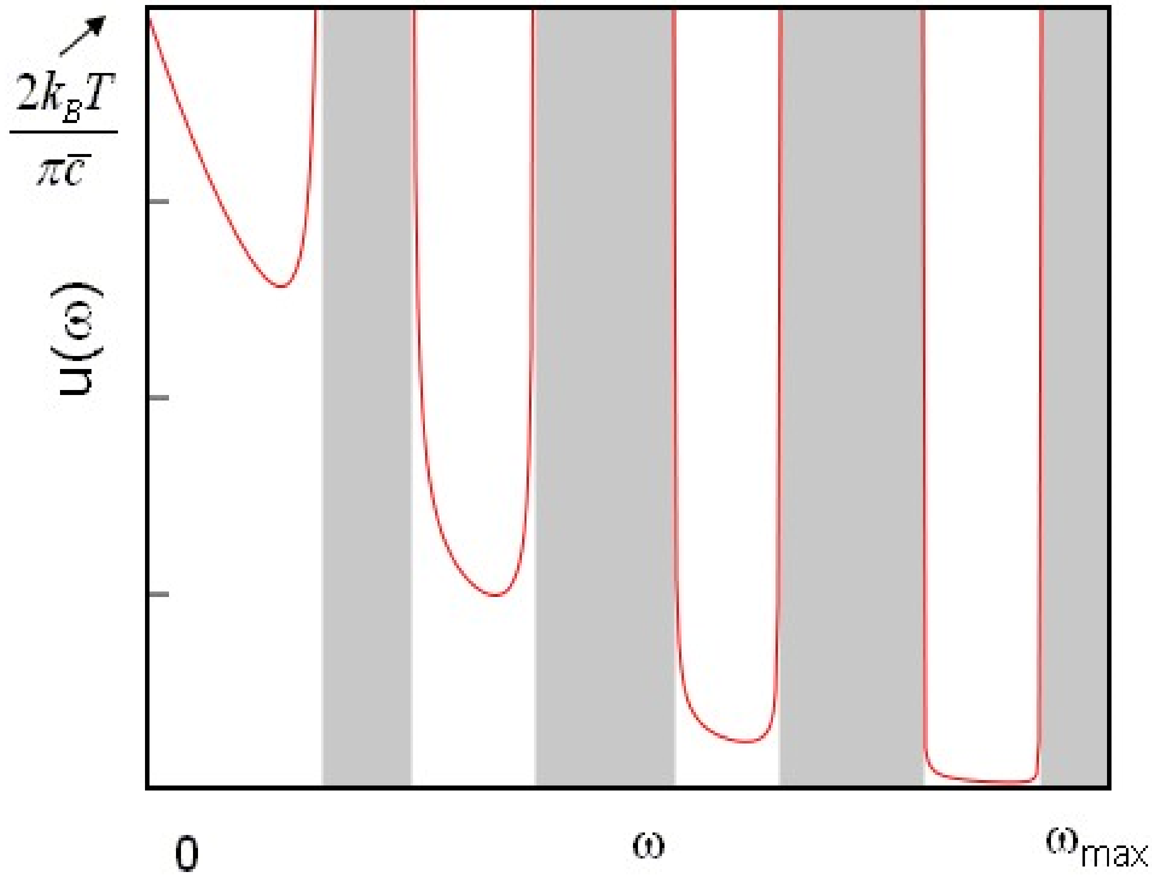




$$D(\omega) = D(k)\frac{dk}{d\omega}$$

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

Energy spectral density



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

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)

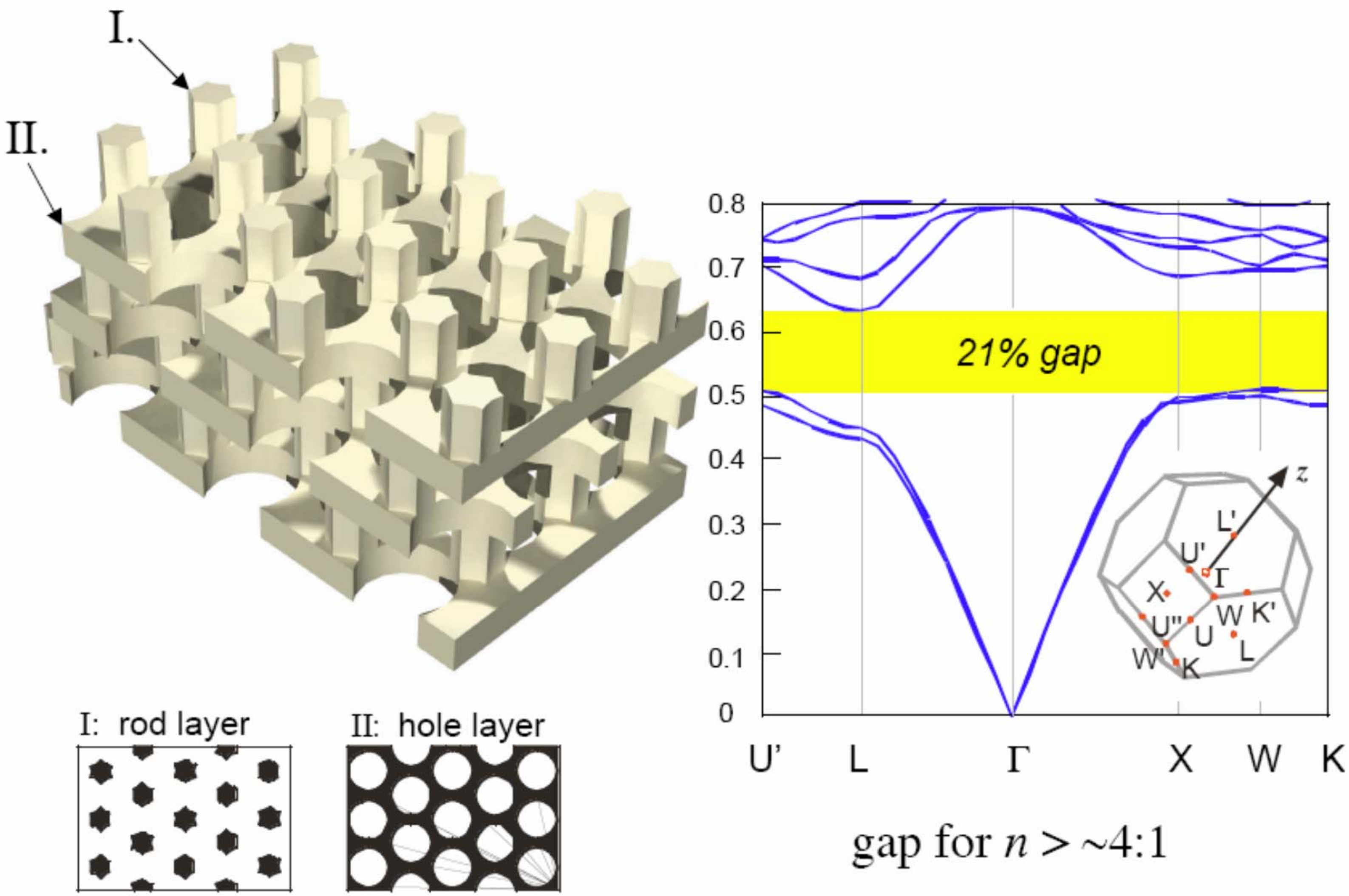
Internal energy density: $$u(T) = \int_0^\infty \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega$$ DoS → u(T)

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)

3d photonic crystal: complete gap , ε=12:1



gap for n > ~4:1

[S. G. Johnson *et al.*, *Appl. Phys. Lett.* **77**, 3490 (2000)]

http://ab-initio.mit.edu/photons/tutorial/L1-bloch.pdf

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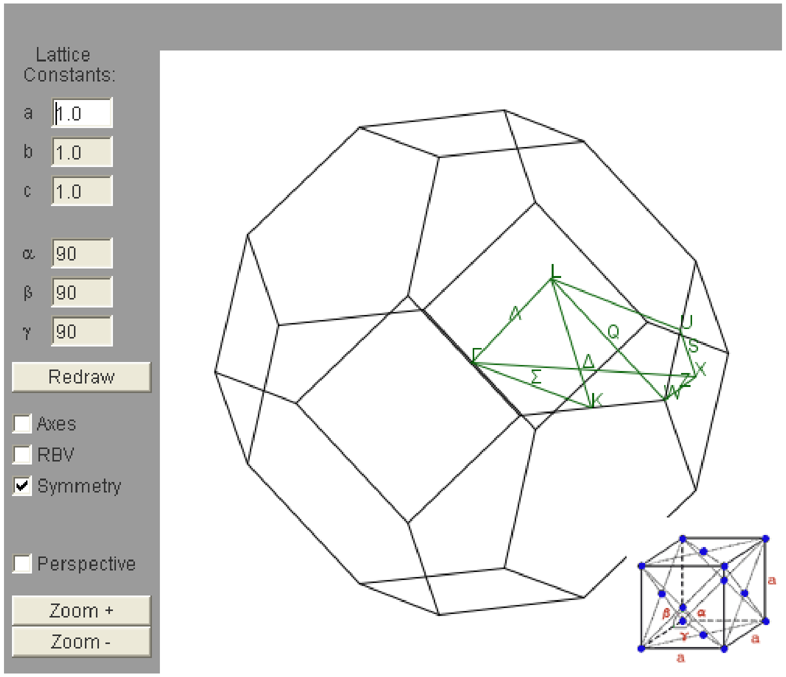
The first Brillouin zone of a face centered cubic lattice



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

Symmetry points (u,v,w)	$[k_x,k_y,k_z]$	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/2*a*,2π/*a*,π/2*a*]	mm2
K: (3/8,3/4,3/8)	[3π/2*a*,3π/2*a*,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*,2*u*,*u*) 0 < *u* < 3/8	mm2
S: (2*u*,1/2+2*u*,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:

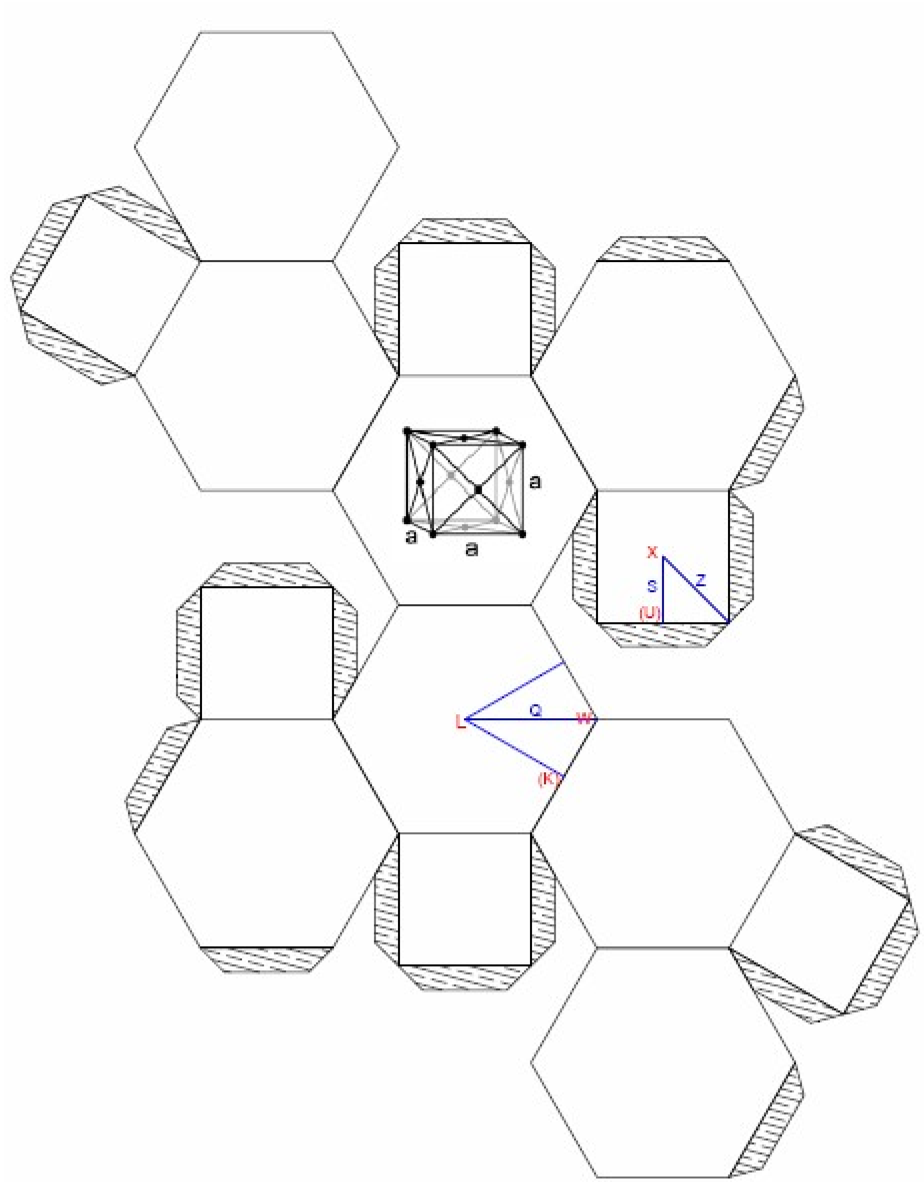
$$\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{z}), \qquad \vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{y}), \qquad \vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{z}),$$

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

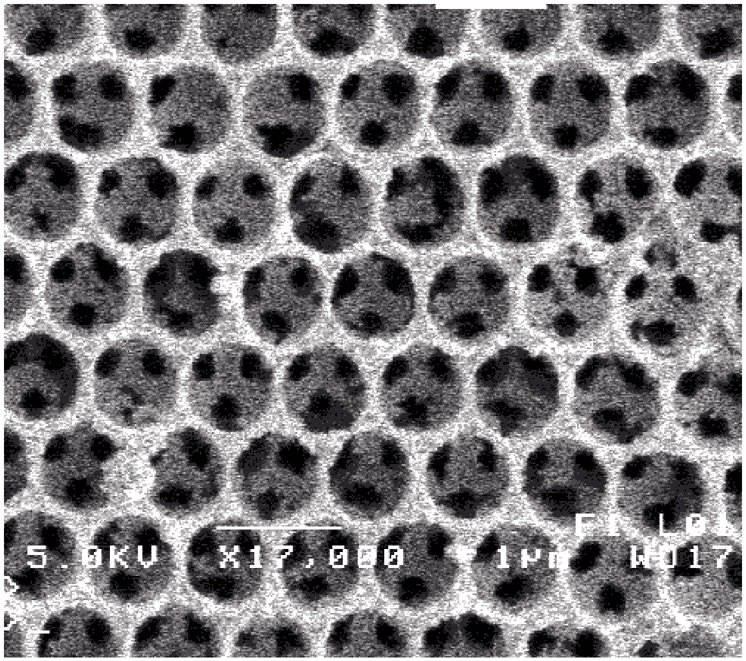
Cut-out patterns for Brillouin zones

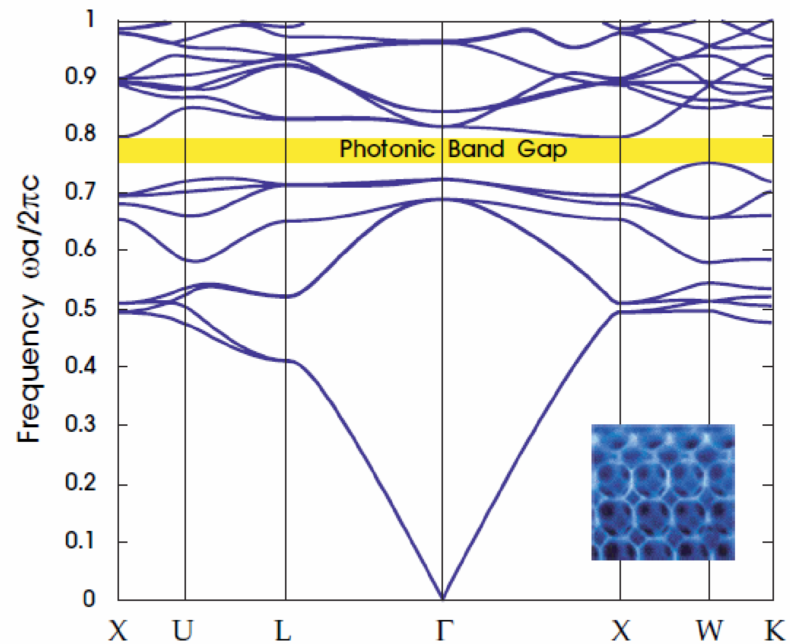
Cut-out patterns to make your own models of the Brillouin zones. The symmetry points are red and the symmetry lines are blue.

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



Inverse opal photonic crystal





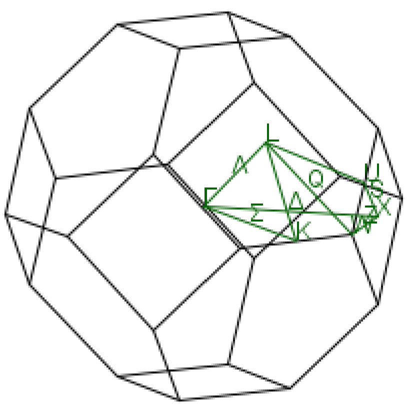


Figure 8: The photonic band structure for the lowest bands of an "inverse opal" structure: a face-centered cubic (fcc) lattice of close-packed air spheres in dielectric ($\varepsilon = 13$). (Inset shows fabricated structure from figure 9.) There is a complete photonic band gap (yellow) between the eighth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