METAgenierie 2017

METAgenierie 2017 : Principles of acoustic metamaterials and their possibilities for the engineering applications

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MODULE CF1 : Dispersion relations – Generalities; PWE et EPWE : Principles

MODULE CF1 : Dispersion relations – Generalities;
PWE and EPWE : Principles.

-Dispersion relations (band structures) in periodic structures

- Plane Wave Expansion (PWE) method

- Extended Plane Wave Expansion (EPWE) method

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OUTLINE

Introduction : Infinite one-dimensional linear chains of atoms (mass-spring model)

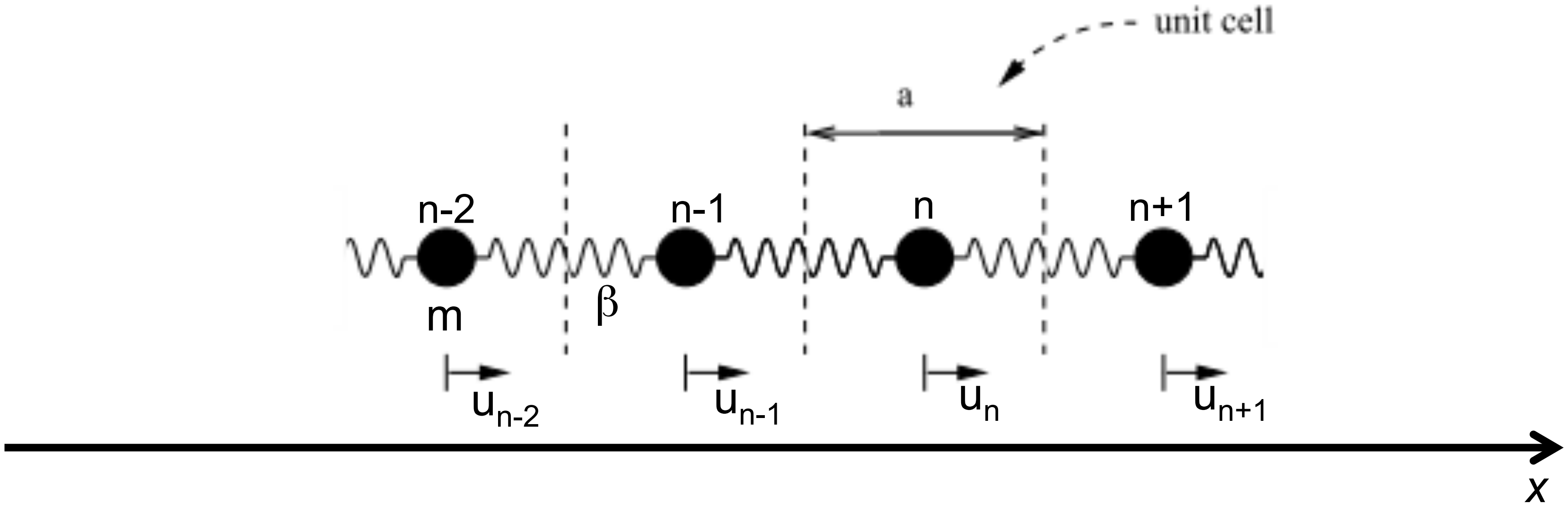
Periodic structures and band structures :

I) Equations of propagation of elastic waves,
Bloch theorem, Fourier series,
PWE method for phononic crystals of infinite extent ("*bulk phononic crystals*"),
numerical code, band structure, pass bands and stop bands,
advantages and drawbacks of the PWE method.

II) Extended PWE method for complex band structures, complex wave vectors,
evanescent waves, examples.

INTRODUCTION

A very simple periodic structure : an infinite one-dimensional linear chain of atoms of identical mass m, connected by springs with (constant) spring constant β



Equilibrium position of atom n is $x_{n,eq}=na$ where a is the distance between two atoms in their equilibrium position.

Atoms are free to move slightly around their respective equilibrium position.

Position, at any date t, of moving atoms is given as $x_n(t)=na+u_n(t)$ with $|u_n(t)| << |x_n(t)|$ and $u_n = x_n - x_{n,eq} \equiv$ displacement of the n^{th} atom from the equilibrium position

a ≡ lattice spacing ≡ periodicity !!!

Newton's second law applied to atom n (interaction between first neighbours)

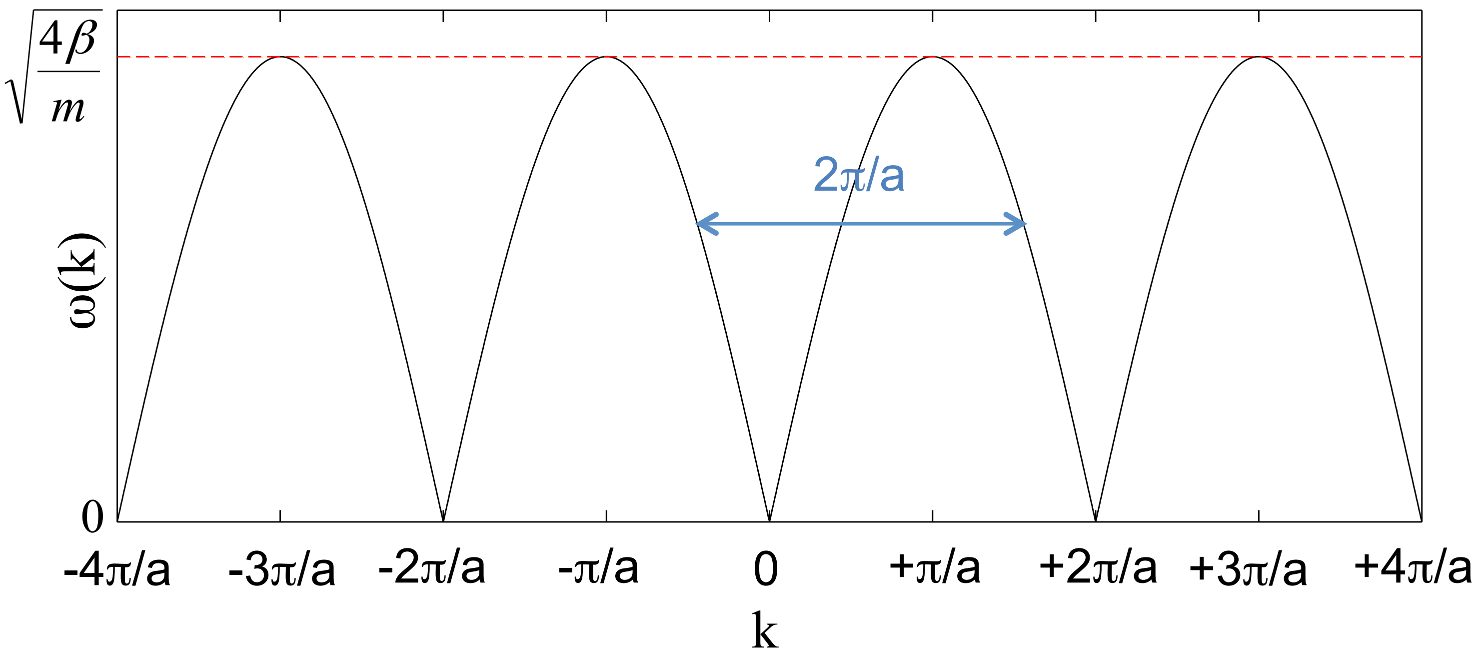
$$\Rightarrow m\frac{d^2u_n}{dt^2} = -\beta(u_n - u_{n-1}) + \beta(u_{n+1} - u_n) = \beta(u_{n+1} + u_{n-1} - 2u_n)$$

Solutions ≡ propagating sinusoidal waves of the form $u_n(n,t) = U_0 e^{i(kna-\omega t)}$

$$\Rightarrow -m\omega^2 = \beta\left(e^{ika} + e^{-ika} - 2\right) = 2\beta(\cos(ka) - 1) = -4\beta\sin^2\left(\frac{ka}{2}\right) \Rightarrow \boxed{\omega(k) = \sqrt{\frac{4\beta}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|}$$

m ≡ mass (kg)
β ≡ spring constant ($N.m^{-1}$)
ω ≡ circular frequency ($rad.s^{-1}$)
a ≡ periodicity of the « direct lattice » (m)
k ≡ wave number (m^{-1}) ↔ « reciprocal lattice »

ω(k) ≡ dispersion relation



$|\sin x|$ is π-periodic $\Rightarrow \left|\sin\left(\frac{ka}{2}\right)\right| = \left|\sin\left(\frac{ka}{2}+\pi\right)\right| = \left|\sin\left(\frac{a}{2}\left(k+\frac{2\pi}{a}\right)\right)\right|$

⇒ ω(k) is a periodic function of k with periodicity G=2π/a

⇒ ω(k+nG)=ω(k), n integer

⇒ A propagation mode of wave number k and a mode with wave number (k+G) are equivalent!!!

G is associated with the «reciprocal lattice» (periodicity 2π/a) of the chain («direct lattice» of periodicity a)

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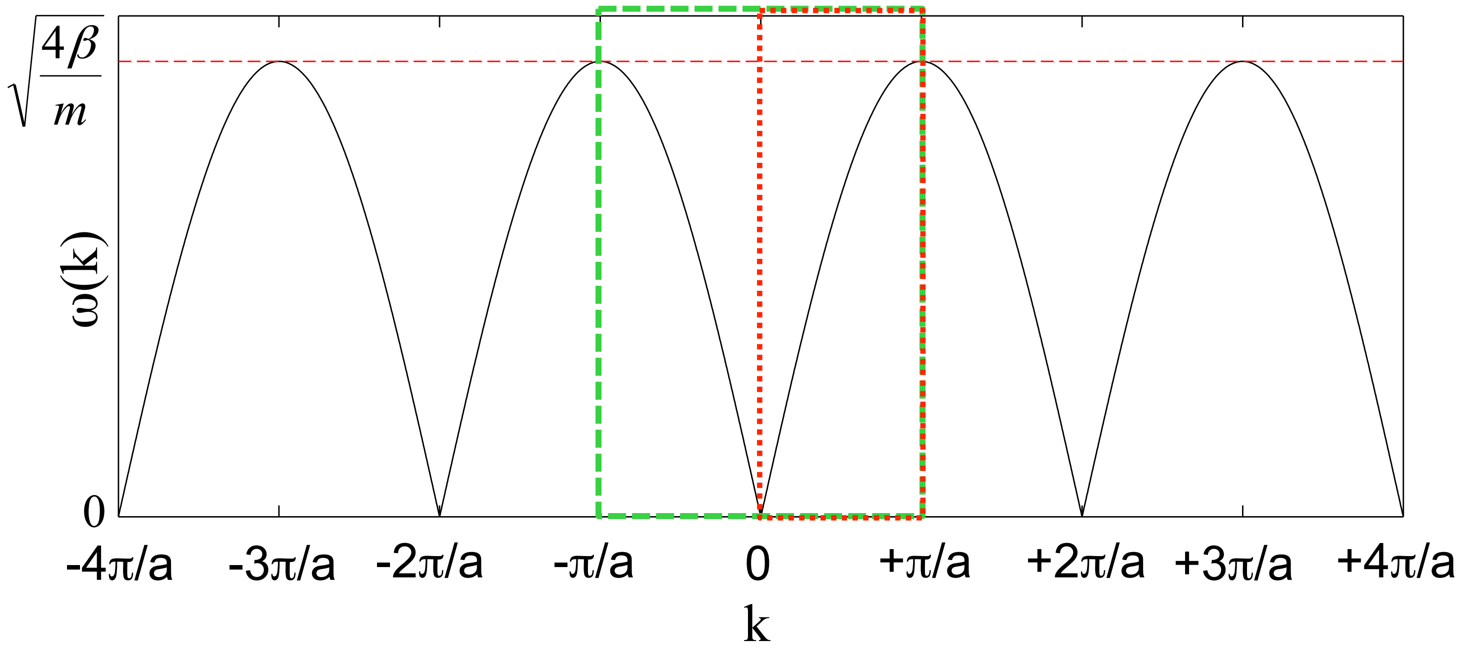
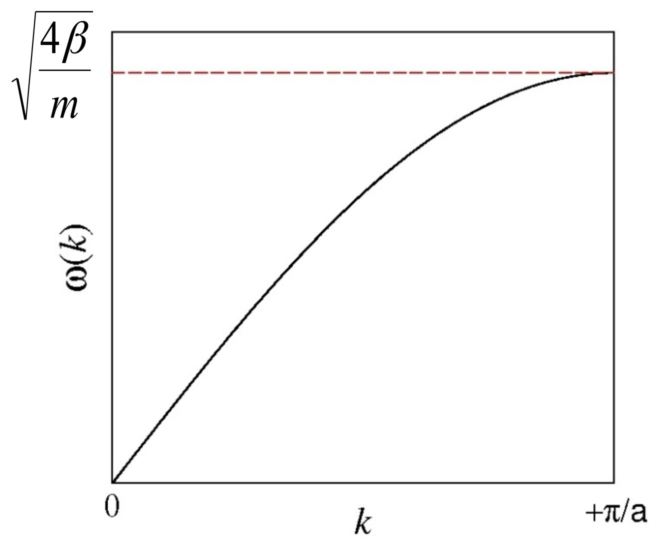


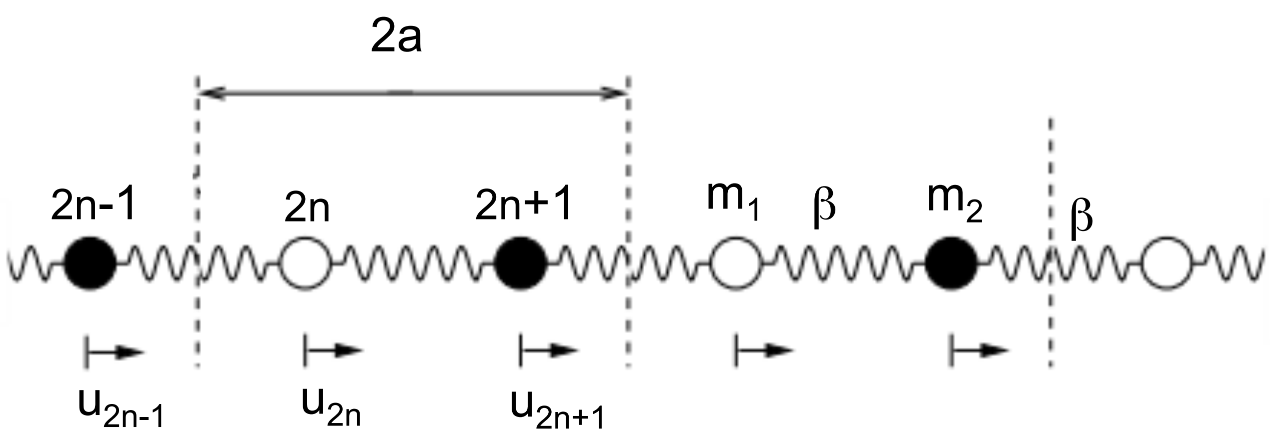
Due to the periodicity of the dispersion relation in the wave number space (reciprocal space), the useful information is contained in the waves with wave numbers lying between the limits $-\pi/a$ and $+\pi/a$

⇔ first Brillouin zone (centered on k=0).

Dispersion relation is also symmetric with respect of the plane k=0, and one may focus the study on wave numbers ranging from 0 to $+\pi/a$ ⇒ Irreducible Brillouin zone



A bit more complicated periodic structure : an infinite one-dimensional linear chain with two atoms of different masses in the unit cell



Assumption : All the springs have the same constant β !!

The equations of motion of two adjacent odd (2n+1) and even (2n) atoms are

$$\begin{cases} m_1 \dfrac{d^2 u_{2n}}{dt^2} = -\beta(u_{2n} - u_{2n-1}) + \beta(u_{2n+1} - u_{2n}) = \beta(u_{2n+1} + u_{2n-1} - 2u_{2n}) \\ m_2 \dfrac{d^2 u_{2n+1}}{dt^2} = -\beta(u_{2n+1} - u_{2n}) + \beta(u_{2n+2} - u_{2n+1}) = \beta(u_{2n+2} + u_{2n} - 2u_{2n+1}) \end{cases}$$

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Solutions ≡ propagating sinusoidal waves of the form $\begin{cases} u_{2n}(n,t) = Ae^{i(k2na-\omega t)} \\ u_{2n+1}(n,t) = Be^{i(k(2n+1)a-\omega t)} \end{cases}$

One obtains a set of two equations with 2 unknowns A and B

$$\begin{cases} -m_1\omega^2 A = \beta\left(Be^{ika} + Be^{-ika} - 2A\right) \\ -m_2\omega^2 B = \beta\left(Ae^{ika} + Ae^{-ika} - 2B\right) \end{cases} \Leftrightarrow \begin{cases} \left(2\beta - m_1\omega^2\right)A - 2\beta\cos(ka)B = 0 \\ 2\beta\cos(ka)A - \left(2\beta - m_2\omega^2\right)B = 0 \end{cases}$$

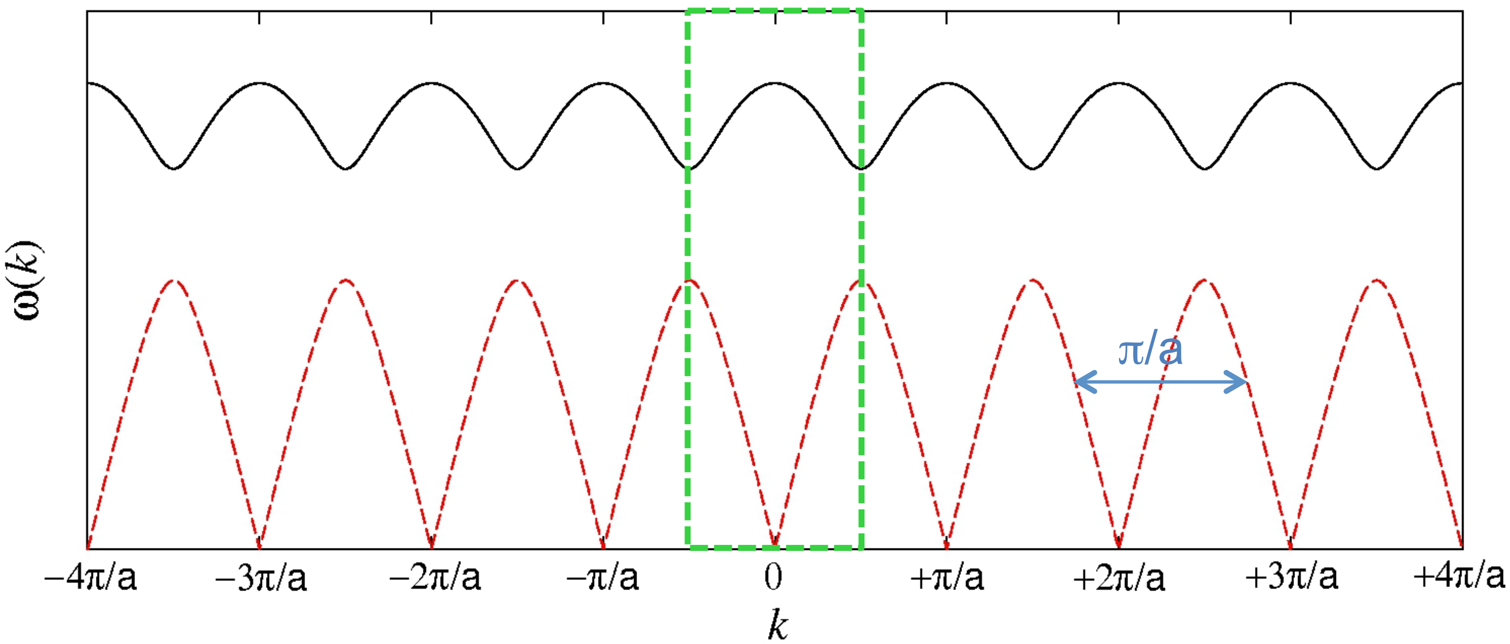
Non-trivial (A=B=0!!!) solutions of this set of equations are obtained if

$$\begin{vmatrix} 2\beta - m_1\omega^2 & -2\beta\cos(ka) \\ 2\beta\cos(ka) & -\left(2\beta - m_2\omega^2\right) \end{vmatrix} = 0 \quad \text{then} \quad \omega^4 - 2\beta\left(\frac{m_1+m_2}{m_1m_2}\right)\omega^2 + \frac{4\beta^2}{m_1m_2}\sin^2(ka) = 0$$

and

$$\omega(k) = \sqrt{\beta\left(\frac{m_1+m_2}{m_1m_2}\right) \pm \sqrt{\beta^2\left(\frac{m_1+m_2}{m_1m_2}\right)^2 - \frac{4\beta^2}{m_1m_2}\sin^2(ka)}}$$

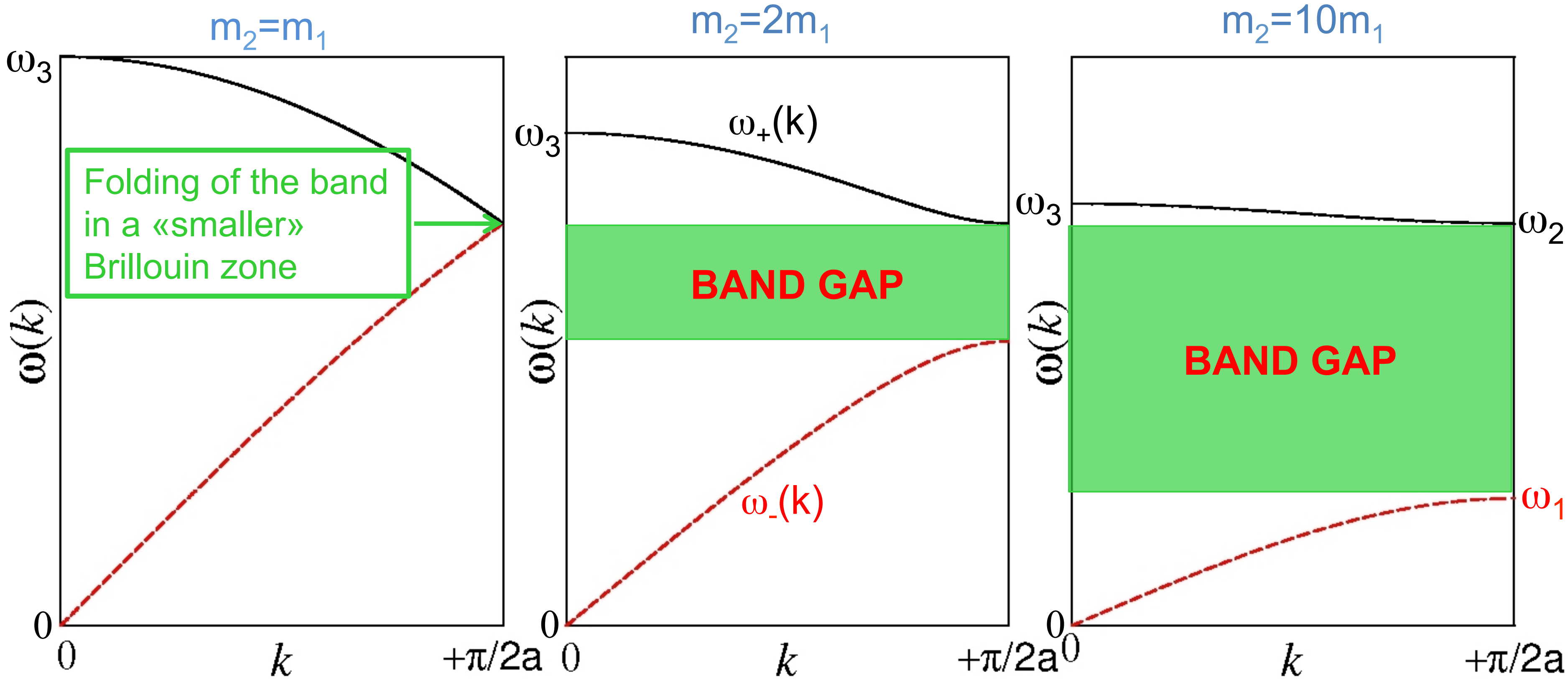
⇒ Two solutions, $\omega_-(k)$ and $\omega_+(k)$, that are periodic in wave number, k, with a period of π/a (due to the dependence with $\sin^2(ka)$ rather than $\sin^2(ka/2)$)



Periodicity of the «direct lattice» =2a

⇒ Periodicity of the «reciprocal lattice» =2π/2a=π/a !

⇒ first Brillouin zone : k∈[-π/2a,+π/2a]



Band structure plotted in the irreducible Brillouin zone : $k \in [0, +\pi/2a]$

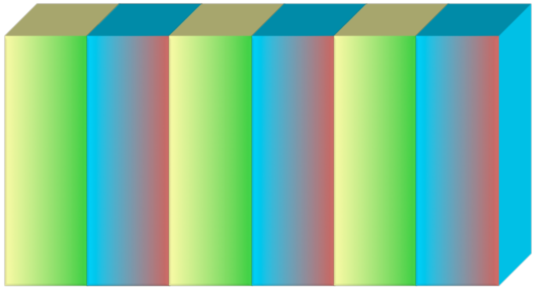
With two different atoms in the unit cell, the band structure exhibits a band gap (or stop band) for $\omega_1 < \omega < \omega_2$. Larger is m_2/m_1, larger is the gap!!!

$$\omega_1 = \sqrt{\frac{2\beta}{m_2}}, \omega_2 = \sqrt{\frac{2\beta}{m_1}}, \omega_3 = \sqrt{\frac{2\beta(m_1 + m_2)}{m_1 . m_2}}$$

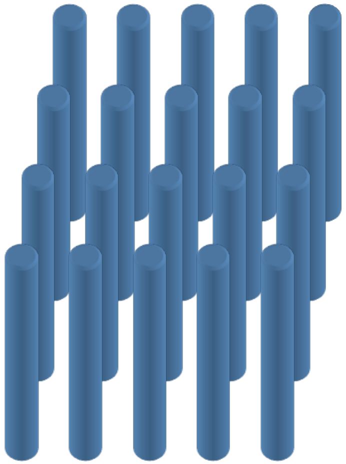
…. much more complicated periodic structures : the **phononic crystals**

Artificial crystals whose physical characteristics (elastic constants and density) are periodic functions of the position (1D, 2D, 3D)

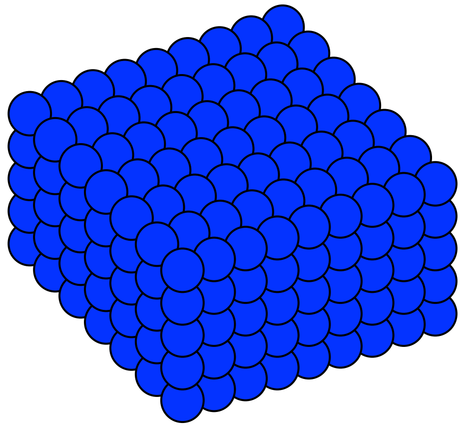
1D: Multilayers materials



2D: Array of cylinders of circular, square, … cross section embedded in a matrix



3D: Array of spheres, cubes, … embedded in a matrix



⇒ Study of such «artificial» crystals can be done using the same «tools» as those developed for «natural crystals» (direct and reciprocal lattices, Brillouin zone, band structures ….)

I) Equations of propagation of elastic waves and the plane waves expansion method.

Equations of propagation of elastic waves in an «inhomogeneous solid» ?

- Inhomogeneous elastic medium of infinite extent along the 3 spatial directions (x_1,x_2,x_3), made of constituent materials of specific crystallographic symmetry (isotropic, cubic, …).

- At every point, $\vec{r}$, the medium is characterized by the material parameters : mass density $\rho(\vec{r})$ and elastic moduli $C_{ijkl}(\vec{r})$

- $C_{ijkl}(\vec{r})$ depend on the crystallographic symmetry of the constituent materials and $C_{ijkl} = C_{jikl}$ and $C_{ijkl} = C_{ijlk}$

-The elements of the stress tensors (T_{ij}) and those of the strain tensors (S_{kl}) are related through the Hooke's law $T_{ij}(\vec{r}) = \sum_{kl} C_{ijkl}(\vec{r}) S_{kl}(\vec{r})$

- Constituent materials are assumed to be linear materials (small strains) and the elements of the strain tensor are expressed as $S_{kl}(\vec{r}) = \frac{1}{2}\left(\frac{\partial u_k(\vec{r})}{\partial x_l} + \frac{\partial u_l(\vec{r})}{\partial x_k}\right)$

where $u_i\,(i=1,2,3)$ refers to the components of the displacement vector $\vec{u}(\vec{r},t)$

$$T_{ij}=\sum_{kl}C_{ijkl}S_{kl}=\sum_{kl}C_{ijkl}\left[\frac{1}{2}\left(\frac{\partial u_k}{\partial x_l}+\frac{\partial u_l}{\partial x_k}\right)\right]=\frac{1}{2}\sum_{kl}C_{ijkl}\frac{\partial u_k}{\partial x_l}+\frac{1}{2}\sum_{kl}C_{ijkl}\frac{\partial u_l}{\partial x_k}$$

$$=\frac{1}{2}\sum_{kl}C_{ijkl}\frac{\partial u_k}{\partial x_l}+\frac{1}{2}\sum_{kl}C_{ijlk}\frac{\partial u_l}{\partial x_k}=\sum_{kl}C_{ijkl}\frac{\partial u_k}{\partial x_l}$$

-For the sake of simplicity, constituent materials are supposed to be of cubic symmetry. In that case, the «matrix » of elastic moduli writes,

$$\overline{\overline{C}}=\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

→

3 independent elastic moduli : C_{11}, C_{12}, C_{44}

For isotropic materials,

$$\begin{cases} C_{12}=C_{11}-2C_{44} \\ C_{11}=\rho V_L^2 \quad \text{and} \quad C_{44}=\rho V_T^2 \end{cases}$$

using the Voigt notation: *pair of indices kl becomes «index» m such as*

ij	11	22	33	23 or 32	31 or 13	12 or 21
m	1	2	3	4	5	6

• <u>EXERCISE</u> : Writes T_{ij} as functions of C_{mn} and u_i ?

$$T_{11} = \sum_{kl} C_{11kl} \frac{\partial u_k}{\partial x_l} = C_{1111}\frac{\partial u_1}{\partial x_1} + C_{1112}\frac{\partial u_1}{\partial x_2} + C_{1113}\frac{\partial u_1}{\partial x_3}$$

$$+ C_{1121}\frac{\partial u_2}{\partial x_1} + C_{1122}\frac{\partial u_2}{\partial x_2} + C_{1123}\frac{\partial u_2}{\partial x_3}$$

$$+ C_{1131}\frac{\partial u_3}{\partial x_1} + C_{1132}\frac{\partial u_3}{\partial x_2} + C_{1133}\frac{\partial u_3}{\partial x_3}$$

$$= C_{11}\frac{\partial u_1}{\partial x_1} + \underbrace{C_{16}}_{0}\frac{\partial u_1}{\partial x_2} + \underbrace{C_{15}}_{0}\frac{\partial u_1}{\partial x_3}$$

$$+ \underbrace{C_{16}}_{0}\frac{\partial u_2}{\partial x_1} + C_{12}\frac{\partial u_2}{\partial x_2} + \underbrace{C_{14}}_{0}\frac{\partial u_2}{\partial x_3}$$

$$+ \underbrace{C_{15}}_{0}\frac{\partial u_3}{\partial x_1} + \underbrace{C_{14}}_{0}\frac{\partial u_3}{\partial x_2} + C_{13}\frac{\partial u_3}{\partial x_3}$$

$$\Rightarrow T_{11} = C_{11}\frac{\partial u_1}{\partial x_1} + C_{12}\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right)$$

In the same way, one obtains

$$T_{12} = \sum_{kl} C_{12kl} \frac{\partial u_k}{\partial x_l} = C_{44}\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) = T_{21}$$

$$T_{13} = \sum_{kl} C_{13kl} \frac{\partial u_k}{\partial x_l} = C_{44}\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right) = T_{31}$$

$$T_{22} = \sum_{kl} C_{22kl} \frac{\partial u_k}{\partial x_l} = C_{11}\frac{\partial u_2}{\partial x_2} + C_{12}\left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_3}{\partial x_3}\right)$$

$$T_{23} = \sum_{kl} C_{23kl} \frac{\partial u_k}{\partial x_l} = C_{44}\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right) = T_{32}$$

$$T_{33} = \sum_{kl} C_{33kl} \frac{\partial u_k}{\partial x_l} = C_{11}\frac{\partial u_3}{\partial x_3} + C_{12}\left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2}\right)$$

- In absence of external forces, Newton's second law leads to the equations of motion

$$\rho(\vec{r})\frac{\partial^2 u_i(\vec{r},t)}{\partial t^2} = \sum_j \frac{\partial T_{ij}(\vec{r})}{\partial x_j} = \sum_j \frac{\partial}{\partial x_j}\left[\sum_{kl} C_{ijkl}(\vec{r})\frac{\partial u_k(\vec{r})}{\partial x_l}\right]$$

and

$$\rho(\vec{r})\frac{\partial^2 u_1(\vec{r},t)}{\partial t^2} = \frac{\partial T_{11}(\vec{r})}{\partial x_1} + \frac{\partial T_{12}(\vec{r})}{\partial x_2} + \frac{\partial T_{13}(\vec{r})}{\partial x_3}$$

$$= \frac{\partial}{\partial x_1}\left(C_{11}(\vec{r})\frac{\partial u_1}{\partial x_1} + C_{12}(\vec{r})\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right)\right) + \frac{\partial}{\partial x_2}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right) + \frac{\partial}{\partial x_3}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)\right)$$

$$\rho(\vec{r})\frac{\partial^2 u_2(\vec{r},t)}{\partial t^2} = \frac{\partial T_{21}(\vec{r})}{\partial x_1} + \frac{\partial T_{22}(\vec{r})}{\partial x_2} + \frac{\partial T_{23}(\vec{r})}{\partial x_3}$$

$$= \frac{\partial}{\partial x_1}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right) + \frac{\partial}{\partial x_2}\left(C_{11}(\vec{r})\frac{\partial u_2}{\partial x_2} + C_{12}(\vec{r})\left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_3}{\partial x_3}\right)\right) + \frac{\partial}{\partial x_3}\left(C_{44}(\vec{r})\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)\right)$$

$$\rho(\vec{r})\frac{\partial^2 u_3(\vec{r},t)}{\partial t^2} = \frac{\partial T_{31}(\vec{r})}{\partial x_1} + \frac{\partial T_{32}(\vec{r})}{\partial x_2} + \frac{\partial T_{33}(\vec{r})}{\partial x_3}$$

$$= \frac{\partial}{\partial x_1}\left(C_{44}(\vec{r})\left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3}\right)\right) + \frac{\partial}{\partial x_2}\left(C_{44}(\vec{r})\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)\right) + \frac{\partial}{\partial x_3}\left(C_{11}(\vec{r})\frac{\partial u_3}{\partial x_3} + C_{12}(\vec{r})\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_1}{\partial x_1}\right)\right)$$

Equations of propagation of elastic waves in an heterogeneous elastic material of infinite extent are three coupled differential equations of order 2

For «periodic» distributions of inhomogeneities, these equations can be solved using the Plane Wave Expansion (PWE) method

Basic principles of the PWE method for infinite phononic crystals

- Direct lattice (DL), of specific geometry, characterized by its unit cell (UC)

- Reciprocal lattice (RL) of vectors $\vec{G}(G_1, G_2, G_3)$ with respect to the basis $(O, \vec{e}_1, \vec{e}_2, \vec{e}_3)$

- One search sinusoidally time varying solutions of the equations of propagation in the form $\vec{u}(\vec{r},t) = \vec{u}(\vec{r}).e^{-i\omega t}$ where ω is the circular frequency

- Due to the periodicity of the structure, the **Bloch-Floquet theorem** states that $\vec{u}(\vec{r})$ can be written in the form $\vec{u}(\vec{r}) = e^{i\vec{K}.\vec{r}}\vec{U}_{\vec{K}}(\vec{r})$ where $\vec{K}(K_1, K_2, K_3)$ is the Bloch wave vector and $\vec{U}_{\vec{K}}(\vec{r})$ has the <u>periodicity of the direct lattice</u>

➡ $\vec{U}_{\vec{K}}(\vec{r})$ can be developped in Fourier series as

$$\vec{U}_{\vec{K}}(\vec{r}) = \sum_{G'} \vec{U}_{\vec{K}}(\vec{G}')e^{i\vec{G}'\cdot\vec{r}} \text{ where } \vec{G}' \in RL$$

➡ $$\vec{u}(\vec{r},t) = e^{i(\vec{K}.\vec{r}-\omega t)} \sum_{G'} \vec{U}_{\vec{K}}(\vec{G}')e^{i\vec{G}'\cdot\vec{r}}$$

-The material parameters, mass density $\rho(\vec{r})$ and elastic moduli $C_{ijkl}(\vec{r})$ are periodic functions of the position i.e. $\rho(\vec{r}) = \rho(\vec{r}+\vec{R})$ and $C_{ijkl}(\vec{r}) = C_{ijkl}(\vec{r}+\vec{R})$ where $\vec{R} \in (\mathrm{DL})$ and can be expanded in Fourier series such as

$$\begin{cases} C_{ijkl}(\vec{r}) = \sum_{G''} C_{ijkl}(\vec{G}'') e^{i\vec{G}''\cdot\vec{r}} \\ \rho(\vec{r}) = \sum_{G''} \rho(\vec{G}'') e^{i\vec{G}''\cdot\vec{r}} \end{cases} \quad \text{where } \vec{G}'' \in (RL)$$

- $\vec{u}(\vec{r},t)$, $\rho(\vec{r})$, $C_{ijkl}(\vec{r})$ in the equations of propagation are then replaced by these expressions …

Equation of propagation for u_1

$$\rho(\vec{r})\frac{\partial^2 u_1(\vec{r},t)}{\partial t^2} =$$

$$= \frac{\partial}{\partial x_1}\left(C_{11}(\vec{r})\frac{\partial u_1}{\partial x_1} + C_{12}(\vec{r})\left(\frac{\partial u_2}{\partial x_2}+\frac{\partial u_3}{\partial x_3}\right)\right) + \frac{\partial}{\partial x_2}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\right) + \frac{\partial}{\partial x_3}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_3}+\frac{\partial u_3}{\partial x_1}\right)\right)$$

Left hand side $\rho(\vec{r})\frac{\partial^2 u_1(\vec{r},t)}{\partial t^2}$ becomes $-\omega^2 e^{i(\vec{K}.\vec{r}-\omega t)}\sum_{\vec{G}',\vec{G}''}\rho(\vec{G}'')U_{1,\vec{K}}(\vec{G}')e^{i(\vec{G}'+\vec{G}'')\vec{r}}$ ….

Multiplication of this term by $e^{-i\vec{G}.\vec{r}}$ and integration over the unit cell

$$\frac{1}{V_{(UC)}}\int_{(UC)} e^{i(\vec{G}'+\vec{G}''-\vec{G}).\vec{r}}\,d\vec{r} = \delta_{\vec{G}'+\vec{G}''-\vec{G},\vec{0}} = \begin{cases}1 \text{ if } (\vec{G}'+\vec{G}''-\vec{G})=\vec{0}\\ 0 \text{ if } (\vec{G}'+\vec{G}''-\vec{G})\neq\vec{0}\end{cases} \Rightarrow \vec{G}''=\vec{G}-\vec{G}'$$

$V_{(UC)}$ ≡ Volume of the unit cell

… and $-\omega^2 e^{i((\vec{K}+\vec{G}).\vec{r}-\omega t)}\sum_{\vec{G}'}\left[\rho(\vec{G}-\vec{G}')\right]U_{1,\vec{K}}(\vec{G}')$

Right hand side

$$\frac{\partial}{\partial x_1}\left(C_{11}(\vec{r})\frac{\partial u_1}{\partial x_1}+C_{12}(\vec{r})\left(\frac{\partial u_2}{\partial x_2}+\frac{\partial u_3}{\partial x_3}\right)\right)+\frac{\partial}{\partial x_2}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)\right)+\frac{\partial}{\partial x_3}\left(C_{44}(\vec{r})\left(\frac{\partial u_1}{\partial x_3}+\frac{\partial u_3}{\partial x_1}\right)\right)$$

becomes ?????

Method

$$u_1(\vec r,t)=e^{i(\vec K.\vec r-\omega t)}\sum_{G'}U_{1,\vec K}(\vec G')e^{i\vec G'\cdot\vec r}=e^{i\omega t}\sum_{G'}U_{1,\vec K}(\vec G')e^{i(\vec K+\vec G')\vec r}$$

with $(\vec K+\vec G')\vec r=(K_1+G'_1)x_1+(K_2+G'_2)x_2+(K_3+G'_3)x_3$

then $$\frac{\partial u_1(\vec r,t)}{\partial x_1}=e^{i(\vec K.\vec r-\omega t)}\sum_{G'}[i(K_1+G'_1)]U_{1,\vec K}(\vec G')e^{i\vec G'\cdot\vec r}$$

$$C_{11}(\vec r)\frac{\partial u_1(\vec r,t)}{\partial x_1}=e^{-i\omega t}\sum_{\vec G',\vec G''}[i(K_1+G'_1)]U_{1,\vec K}(\vec G')C_{11}(\vec G'')e^{i(\vec K+\vec G'+\vec G'')\vec r}$$

$$\frac{\partial}{\partial x_1}\left[C_{11}(\vec r)\frac{\partial u_1(\vec r,t)}{\partial x_1}\right]=-e^{-i\omega t}\sum_{\vec G',\vec G''}[(K_1+G'_1)(K_1+G'_1+G_1'')]U_{1,\vec K}(\vec G')C_{11}(\vec G'')e^{i(\vec K+\vec G'+\vec G'')\vec r}$$

$$=-e^{i(\vec K.\vec r-\omega t)}\sum_{\vec G',\vec G''}[(K_1+G'_1)(K_1+G'_1+G_1'')]U_{1,\vec K}(\vec G')C_{11}(\vec G'')e^{i(\vec G'+\vec G'')\vec r}$$

Multiplication of all these terms by $e^{-i\vec G.\vec r}$ *and integration of all these terms over the unit cell*

⇒ $\frac{\partial}{\partial x_1}\left[C_{11}(\vec r)\frac{\partial u_1(\vec r,t)}{\partial x_1}\right]$ becomes

$$-e^{i((\vec K+\vec G).\vec r-\omega t)}\sum_{G'}[(K_1+G'_1)(K_1+G_1)C_{11}(\vec G-\vec G')]U_{1,\vec K}(\vec G')$$

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After lengthy algebra (!!!), one obtains

$$\begin{cases} \omega^2 \sum_{G'} B^{(11)}_{\vec{G},\vec{G}'} U_{1,\vec{K}}\left(\vec{G}'\right) = \sum_{G'} \left\{ U_{1,\vec{K}}\left(\vec{G}'\right) A^{(11)}_{\vec{G},\vec{G}'} + U_{2,\vec{K}}\left(\vec{G}'\right) A^{(12)}_{\vec{G},\vec{G}'} + U_{3,\vec{K}}\left(\vec{G}'\right) A^{(13)}_{\vec{G},\vec{G}'} \right\} \\ \omega^2 \sum_{G'} B^{(22)}_{\vec{G},\vec{G}'} U_{2,\vec{K}}\left(\vec{G}'\right) = \sum_{G'} \left\{ U_{1,\vec{K}}\left(\vec{G}'\right) A^{(21)}_{\vec{G},\vec{G}'} + U_{2,\vec{K}}\left(\vec{G}'\right) A^{(22)}_{\vec{G},\vec{G}'} + U_{3,\vec{K}}\left(\vec{G}'\right) A^{(23)}_{\vec{G},\vec{G}'} \right\} \\ \omega^2 \sum_{G'} B^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{G'} \left\{ U_{1,\vec{K}}\left(\vec{G}'\right) A^{(31)}_{\vec{G},\vec{G}'} + U_{2,\vec{K}}\left(\vec{G}'\right) A^{(32)}_{\vec{G},\vec{G}'} + U_{3,\vec{K}}\left(\vec{G}'\right) A^{(33)}_{\vec{G},\vec{G}'} \right\} \end{cases}$$

where

$$
\begin{cases}
B^{(11)}_{\vec{G},\vec{G}'} = B^{(22)}_{\vec{G},\vec{G}'} = B^{(33)}_{\vec{G},\vec{G}'} = \rho\left(\vec{G}-\vec{G}'\right) \\
\\
A^{(11)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)\left(G_1+K_1\right)\left(G'_1+K_1\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[\left(G_2+K_2\right)\left(G'_2+K_2\right)+\left(G_3+K_3\right)\left(G'_3+K_3\right)\right] \\
A^{(12)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)\left(G_1+K_1\right)\left(G'_2+K_2\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left(G'_1+K_1\right)\left(G_2+K_2\right) \\
A^{(13)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)\left(G_1+K_1\right)\left(G'_3+K_3\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left(G'_1+K_1\right)\left(G_3+K_3\right) \\
\\
A^{(21)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)\left(G'_1+K_1\right)\left(G_2+K_2\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left(G'_2+K_2\right)\left(G_1+K_1\right) \\
A^{(22)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)\left(G_2+K_2\right)\left(G'_2+K_2\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[\left(G_1+K_1\right)\left(G'_1+K_1\right)+\left(G_3+K_3\right)\left(G'_3+K_3\right)\right] \\
A^{(23)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)\left(G'_3+K_3\right)\left(G_2+K_2\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left(G'_2+K_2\right)\left(G_3+K_3\right) \\
\\
A^{(31)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)\left(G'_1+K_1\right)\left(G_3+K_3\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left(G_1+K_1\right)\left(G'_3+K_3\right) \\
A^{(32)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)\left(G'_2+K_2\right)\left(G_3+K_3\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left(G_2+K_2\right)\left(G'_3+K_3\right) \\
A^{(33)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)\left(G_3+K_3\right)\left(G'_3+K_3\right) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[\left(G_1+K_1\right)\left(G'_1+K_1\right)+\left(G'_2+K_2\right)\left(G_2+K_2\right)\right]
\end{cases}
$$

After Fourier transform, the equations of propagation can be rewritten as a standard generalized eigenvalues equation in the form

$$\omega^2 \begin{pmatrix} B^{(11)}_{\vec{G},\vec{G}'} & 0 & 0 \\ 0 & B^{(22)}_{\vec{G},\vec{G}'} & 0 \\ 0 & 0 & B^{(33)}_{\vec{G},\vec{G}'} \end{pmatrix} \begin{pmatrix} U_{1,\vec{K}}(\vec{G}') \\ U_{2,\vec{K}}(\vec{G}') \\ U_{3,\vec{K}}(\vec{G}') \end{pmatrix} = \begin{pmatrix} A^{(11)}_{\vec{G},\vec{G}'} & A^{(12)}_{\vec{G},\vec{G}'} & A^{(13)}_{\vec{G},\vec{G}'} \\ A^{(21)}_{\vec{G},\vec{G}'} & A^{(22)}_{\vec{G},\vec{G}'} & A^{(23)}_{\vec{G},\vec{G}'} \\ A^{(31)}_{\vec{G},\vec{G}'} & A^{(32)}_{\vec{G},\vec{G}'} & A^{(33)}_{\vec{G},\vec{G}'} \end{pmatrix} \begin{pmatrix} U_{1,\vec{K}}(\vec{G}') \\ U_{2,\vec{K}}(\vec{G}') \\ U_{3,\vec{K}}(\vec{G}') \end{pmatrix}$$

or $$\omega^2 \overleftrightarrow{B}.\vec{U}_{\vec{K}} = \overleftrightarrow{A}.\vec{U}_{\vec{K}}$$

where $\overleftrightarrow{A}$ and $\overleftrightarrow{B}$ are square matrices whose size depends on the number of reciprocal lattice vectors $\vec{G}$ taken into account in the Fourier series.

For a fixed value of $\vec{K}$ the numerical resolution of this eigenvalue equation is performed for $\vec{K}$ describing the contour of the irreducible Brillouin zone of the array of inclusions.

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Question : what is the meaning of terms of the form $\eta(\vec{G}-\vec{G}')$ in the Fourier transformed equations of propagation?

$$\eta(\vec{r}) = \sum_{G} \eta(\vec{G}) e^{i\vec{G}\cdot\vec{r}} \quad \text{where } \vec{G} \in (RL)$$

Fourier coefficients
of the Fourier series

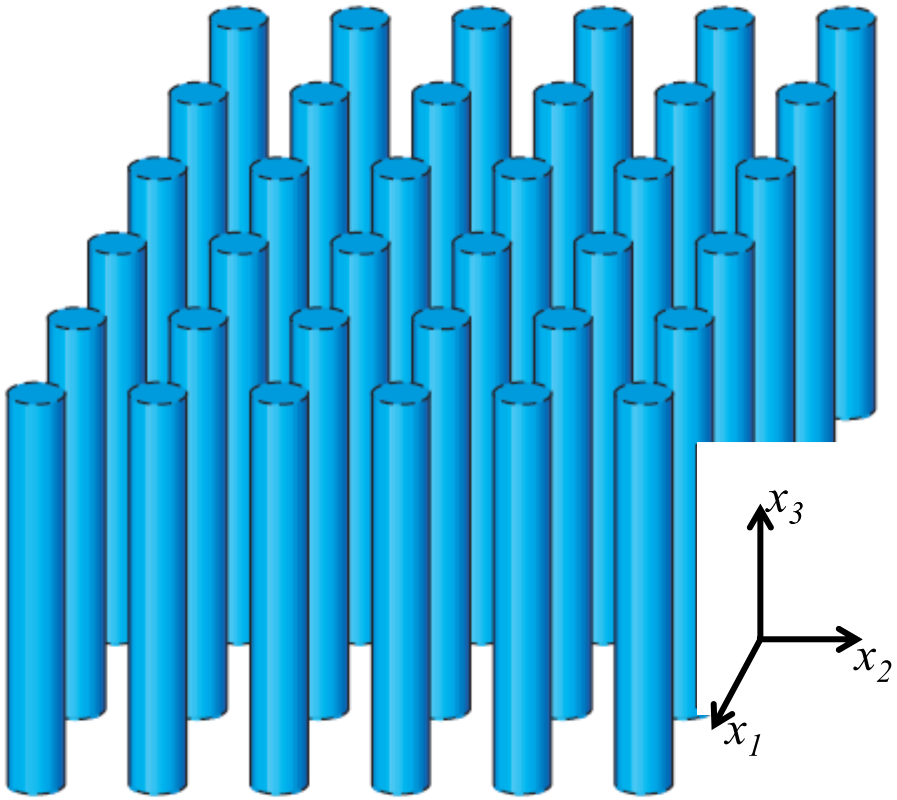
$$\eta(\vec{G}) = \frac{1}{V_{(uc)}} \int_{(UC)} \eta(\vec{r}).e^{-i\vec{G}.\vec{r}}.d\vec{r}$$

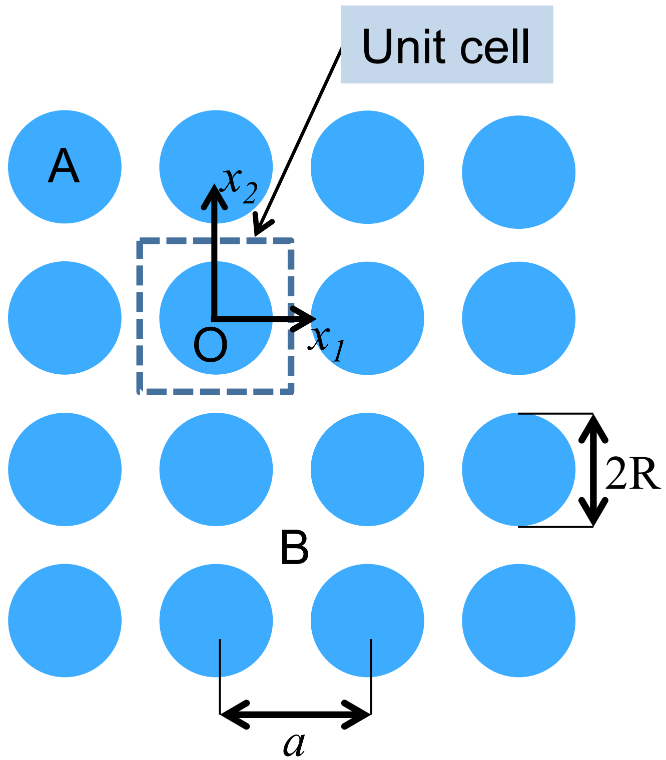
Calculation of $\eta(\vec{G})$?

In the particular case of two-dimensional phononic crystals

TWO-DIMENSIONAL PHONONIC CRYSTALS

Array of cylinders of circular, square, … cross section embedded in a matrix





A ≡ Constituent material of the inclusions
B ≡ Constituent material of the matrix

Hypothesis

-Infinite cylinders along the x_3 direction

⇒Translational symmetry along the x_3 direction

⇒ All quantities (materials parameters, displacement field) independent of x_3

⇒This is a «purely» 2D problem

⇒$G_3=G'_3=0$ and $K_3=0$

Then ……

$$
\begin{cases}
B^{(11)}_{\vec{G},\vec{G}'} = B^{(22)}_{\vec{G},\vec{G}'} = B^{(33)}_{\vec{G},\vec{G}'} = \rho\left(\vec{G}-\vec{G}'\right) \\
\\
A^{(11)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)(G_1+K_1)(G'_1+K_1) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_2+K_2)(G'_2+K_2)\right] \\
A^{(12)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G_1+K_1)(G'_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)(G'_1+K_1)(G_2+K_2) \\
A^{(13)}_{\vec{G},\vec{G}'} = 0 \\
\\
A^{(21)}_{\vec{G},\vec{G}'} = C_{12}\left(\vec{G}-\vec{G}'\right)(G'_1+K_1)(G_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)(G'_2+K_2)(G_1+K_1) \\
A^{(22)}_{\vec{G},\vec{G}'} = C_{11}\left(\vec{G}-\vec{G}'\right)(G_2+K_2)(G'_2+K_2) + C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1)\right] \\
A^{(23)}_{\vec{G},\vec{G}'} = 0 \\
\\
A^{(31)}_{\vec{G},\vec{G}'} = 0 \\
A^{(32)}_{\vec{G},\vec{G}'} = 0 \\
A^{(33)}_{\vec{G},\vec{G}'} = C_{44}\left(\vec{G}-\vec{G}'\right)\left[(G_1+K_1)(G'_1+K_1) + (G'_2+K_2)(G_2+K_2)\right]
\end{cases}
$$

and

$$\omega^2 \begin{pmatrix} B^{(11)}_{\vec{G},\vec{G}'} & 0 & 0 \\ 0 & B^{(22)}_{\vec{G},\vec{G}'} & 0 \\ 0 & 0 & B^{(33)}_{\vec{G},\vec{G}'} \end{pmatrix} \begin{pmatrix} U_{1,\vec{K}}(\vec{G}') \\ U_{2,\vec{K}}(\vec{G}') \\ U_{3,\vec{K}}(\vec{G}') \end{pmatrix} = \begin{pmatrix} A^{(11)}_{\vec{G},\vec{G}'} & A^{(12)}_{\vec{G},\vec{G}'} & 0 \\ A^{(21)}_{\vec{G},\vec{G}'} & A^{(22)}_{\vec{G},\vec{G}'} & 0 \\ 0 & 0 & A^{(33)}_{\vec{G},\vec{G}'} \end{pmatrix} \begin{pmatrix} U_{1,\vec{K}}(\vec{G}') \\ U_{2,\vec{K}}(\vec{G}') \\ U_{3,\vec{K}}(\vec{G}') \end{pmatrix}$$

These 2 matrices are "super-diagonal" and one can separate this matrix equation into two independent uncoupled eigen-values equations

$$\omega^2 \begin{pmatrix} B^{(11)}_{\vec{G},\vec{G}'} & 0 \\ 0 & B^{(22)}_{\vec{G},\vec{G}'} \end{pmatrix} \begin{pmatrix} U_{1,\vec{K}}(\vec{G}') \\ U_{2,\vec{K}}(\vec{G}') \end{pmatrix} = \begin{pmatrix} A^{(11)}_{\vec{G},\vec{G}'} & A^{(12)}_{\vec{G},\vec{G}'} \\ A^{(21)}_{\vec{G},\vec{G}'} & A^{(22)}_{\vec{G},\vec{G}'} \end{pmatrix} \begin{pmatrix} U_{1,\vec{K}}(\vec{G}') \\ U_{2,\vec{K}}(\vec{G}') \end{pmatrix}$$

↔ x_1x_2 (or XY) vibration modes polarized in the transverse plane (x_1Ox_2)

$$\omega^2 \sum_{G'} B^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}(\vec{G}') = \sum_{G'} A^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}(\vec{G}')$$

↔ x_3 or (Z) vibration modes with a displacement field along the x_3 direction

Calculation of $\eta(\vec{G}) = \frac{1}{V_{(uc)}} \int\limits_{(UC)} \eta(\vec{r}).e^{-i\vec{G}.\vec{r}}.d\vec{r}$

For two-dimensional phononic crystals, this equation becomes

$$\eta(\vec{G}) = \frac{1}{\Sigma_{(uc)}} \int\limits_{(UC)} \eta(\vec{r}).e^{-i\vec{G}.\vec{r}}.d\vec{r}$$

where $\Sigma_{(UC)}$ is the area of the two-dimensional unit cell in the (x_1Ox_2) plane

$$\eta(\vec{G}) = \frac{1}{\Sigma_{(UC)}} \iint\limits_{(UC)} \eta(\vec{r})d^2\vec{r} = \frac{1}{\Sigma_{(UC)}} \left\{ \iint\limits_{(A_{(UC)})} \eta_A d^2\vec{r} + \iint\limits_{(B_{(UC)})} \eta_B d^2\vec{r} \right\}$$

$$= \frac{1}{\Sigma_{(UC)}} \iint\limits_{(A_{(UC)})} \eta_A e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} - \frac{1}{\Sigma_{(UC)}} \iint\limits_{(A_{(UC)})} \eta_B e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \frac{1}{\Sigma_{(UC)}} \iint\limits_{(A_{(UC)})} \eta_B e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \frac{1}{\Sigma_{(UC)}} \iint\limits_{(B_{(UC)})} \eta_B e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r}$$

$$= \frac{1}{\Sigma_{(UC)}} \iint\limits_{(A_{(UC)})} \eta_A e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} - \frac{1}{\Sigma_{(UC)}} \iint\limits_{(A_{(UC)})} \eta_B e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \eta_B \left\{ \frac{1}{\Sigma_{(UC)}} \iint\limits_{(UC)} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} \right\}$$

$$= \frac{1}{\Sigma_{(UC)}}(\eta_A - \eta_B) \iint_{(A_{(UC)})} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \eta_B \left\{ \frac{1}{\Sigma_{(UC)}} \iint_{(UC)} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} \right\}.$$

but $$\frac{1}{\Sigma_{(UC)}} \iint_{(UC)} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} = \delta_{\vec{G},\vec{0}} = \begin{cases} 1 \text{ if } \vec{G} = \vec{0} \\ 0 \text{ if } \vec{G} \neq \vec{0} \end{cases}$$

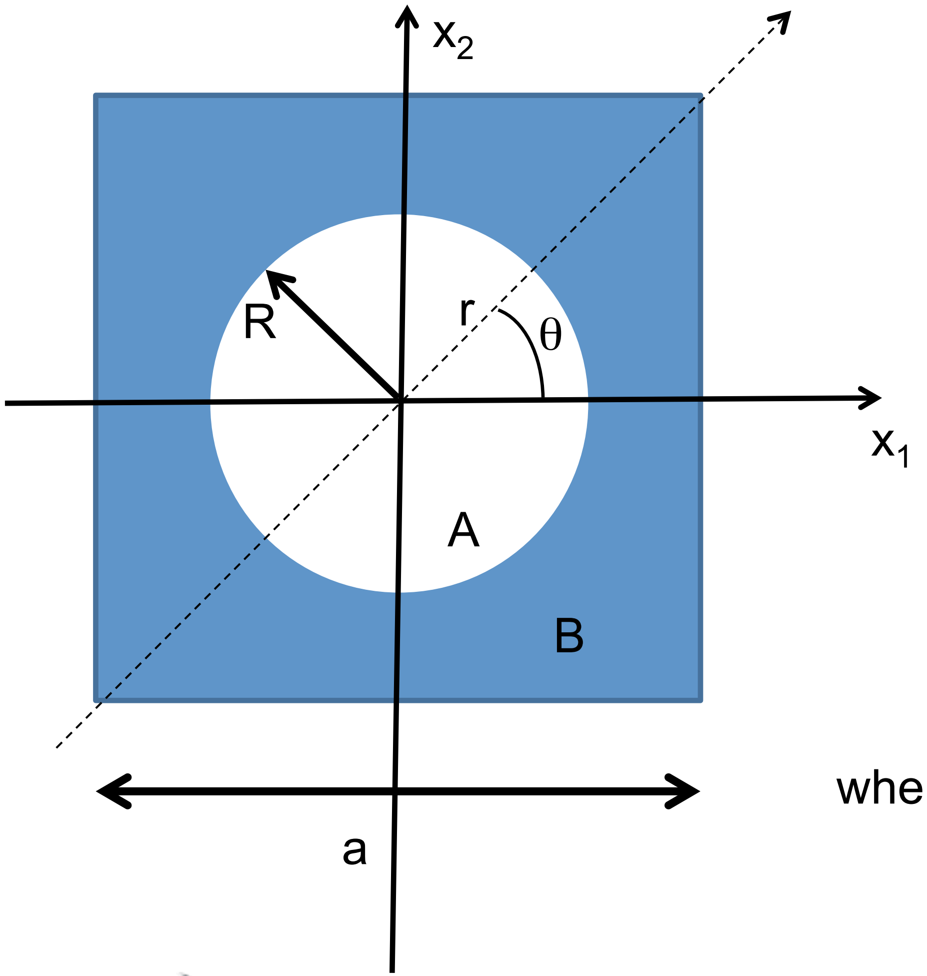
$$\Rightarrow \eta(\vec{G}) = (\eta_A - \eta_B)\frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r} + \eta_B \delta_{\vec{G},\vec{0}}$$

$$\Rightarrow \eta(\vec{G}) = (\eta_A - \eta_B)F(\vec{G}) + \eta_B \delta_{\vec{G},\vec{0}}$$ where $$F(\vec{G}) = \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r}$$ ≡ Structure Factor

depends on the geometry of the inclusions …

Example : Square array (lattice parameter a), of cylinders (circular cross section) of radius R made of material A

⇒ Unit cell = square of side length a



Using polar coordinates (r,θ)

$$F(\vec{G}) = \frac{1}{a^2}\int_0^R \int_0^{2\pi} e^{-iG\cdot r\cos\theta} r dr d\theta$$

$$= \frac{1}{a^2}\int_0^R 2\pi r dr J_0(Gr)$$

$$= \frac{2\pi}{a^2G^2}\int_0^{G_{//}R} (Gr) J_0(Gr) d(Gr)$$

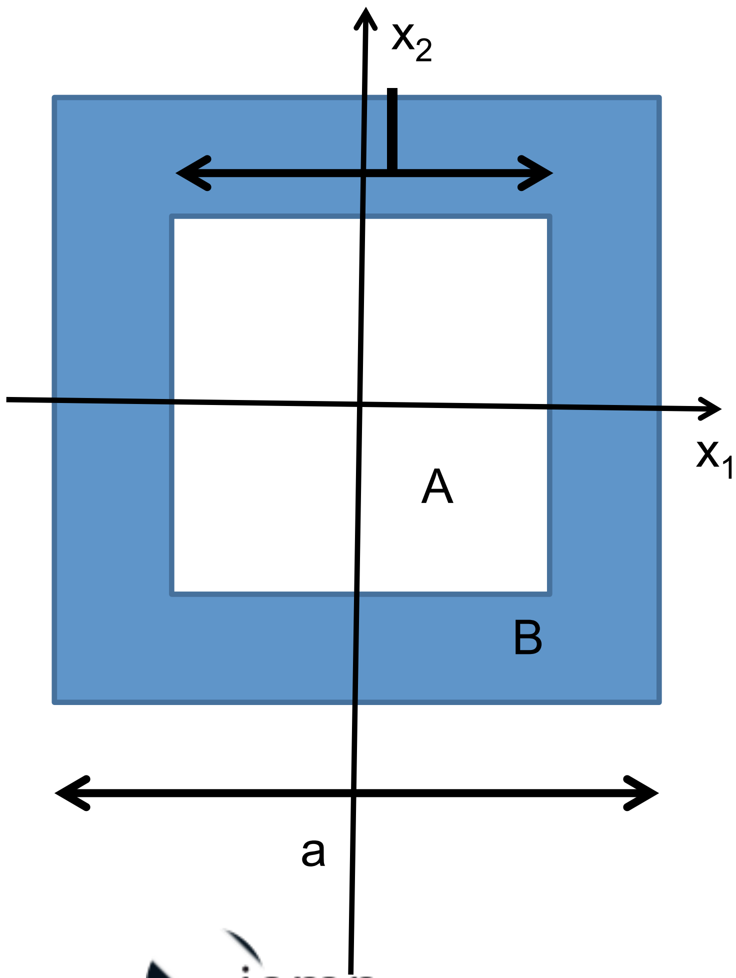
$$= \frac{2\pi}{a^2G^2} GR.J_1(GR) = 2f\frac{J_1(GR)}{GR}$$

where $f = \pi\left(\frac{R}{a}\right)^2 \equiv \text{filling factor};\ 0 \le f \le \frac{\pi}{4}$

$G = \left\|\vec{G}\right\| = \sqrt{G_1^2 + G_2^2}$

J_0 and J_1 are Bessel functions of the first kind of orders 0 and 1

Exercises : Calculate the structure factor for cylinders of square cross section of side length l



$$F(\vec{G}) = \frac{1}{a^2} \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} e^{-iG_1 \cdot x_1} dx_1 \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} e^{-iG_2 \cdot x_2} dx_2$$

$$= \frac{1}{a^2} \left[\frac{e^{-iG_1 \cdot \frac{\ell}{2}} - e^{+iG_1 \cdot \frac{\ell}{2}}}{-iG_1} \right] \left[\frac{e^{-iG_2 \cdot \frac{\ell}{2}} - e^{+iG_2 \cdot \frac{\ell}{2}}}{-iG_2} \right]$$

$$= \frac{1}{a^2} \left[\frac{2i \sin\left(G_1 \cdot \frac{\ell}{2}\right)}{iG_1} \right] \left[\frac{2i \sin\left(G_2 \cdot \frac{\ell}{2}\right)}{iG_2} \right]$$

$$= \frac{1}{a^2} \left[\ell \frac{\sin\left(G_1 \cdot \frac{\ell}{2}\right)}{G_1 \cdot \frac{\ell}{2}} \right] \left[\ell \frac{\sin\left(G_2 \cdot \frac{\ell}{2}\right)}{G_2 \cdot \frac{\ell}{2}} \right]$$

$$= f \left[\frac{\sin\left(G_1 \cdot \frac{\ell}{2}\right)}{G_1 \cdot \frac{\ell}{2}} \right] \left[\frac{\sin\left(G_2 \cdot \frac{\ell}{2}\right)}{G_2 \cdot \frac{\ell}{2}} \right] \quad \text{with } f = \left(\frac{\ell}{a}\right)^2 \text{ and } 0 \le f \le 1$$

$$\eta(\vec{G}) = (\eta_A - \eta_B)F(\vec{G}) + \eta_B \delta_{\vec{G},\vec{0}} \quad \text{where } F(\vec{G}) = \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} e^{-i\vec{G}\cdot\vec{r}} d^2\vec{r}$$

$$\text{If } \vec{G} = \vec{0}, \eta(\vec{G} = \vec{0}) = (\eta_A - \eta_B)F(\vec{G} = \vec{0}) + \eta_B$$

$$\text{and } F(\vec{G} = \vec{0}) = \frac{1}{\Sigma_{(UC)}} \iint_{(A_{(UC)})} d^2\vec{r} = \frac{1}{\Sigma_{(UC)}} . \left(\begin{array}{c} \text{inclusion} \\ \text{area } (\pi R^2 \text{ or } \ell^2) \end{array} \right) = f$$

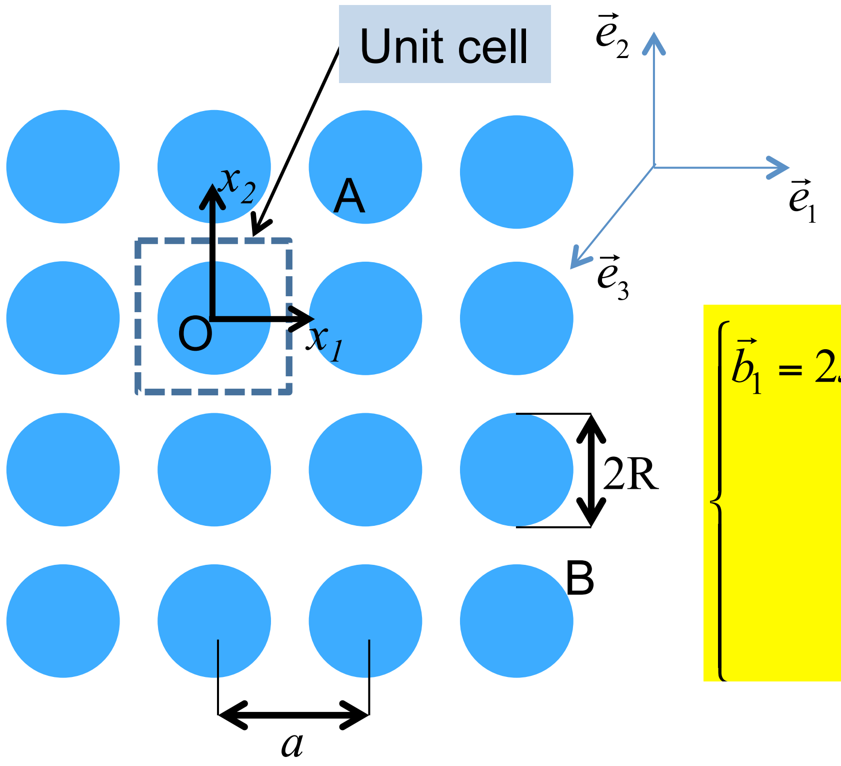
$$\text{then } \eta(\vec{G} = \vec{0}) = (\eta_A - \eta_B)f + \eta_B = \eta_A f + (1 - \eta_B)f = \overline{\eta} \equiv \text{Average value of } \eta \text{ on the unit cell}$$

$$\text{If } \vec{G} \neq \vec{0}, \eta(\vec{G} \neq \vec{0}) = (\eta_A - \eta_B)F(\vec{G} \neq \vec{0})$$

$$\eta(\vec{G}) = (\eta_A - \eta_B)F(\vec{G}) + \eta_B \delta_{\vec{G},\vec{0}} = \begin{cases} \overline{\eta} = f\eta_A + (1 - \mathrm{f})\eta_\mathrm{B} \text{ if } \vec{G} = \vec{0} \\ (\eta_\mathrm{A} - \eta_B)F(\vec{G} \neq \vec{0}) \text{ if } \vec{G} \neq \vec{0} \end{cases}$$

NUMERICAL IMPLEMENTATION:

Particular case of the Z modes in a square array of circular cylinders



Direct lattice of primitive vectors

$$\left(\vec{a}_1 = a\vec{e}_1, \vec{a}_2 = a\vec{e}_2, \vec{a}_3 = \vec{e}_3\right)$$

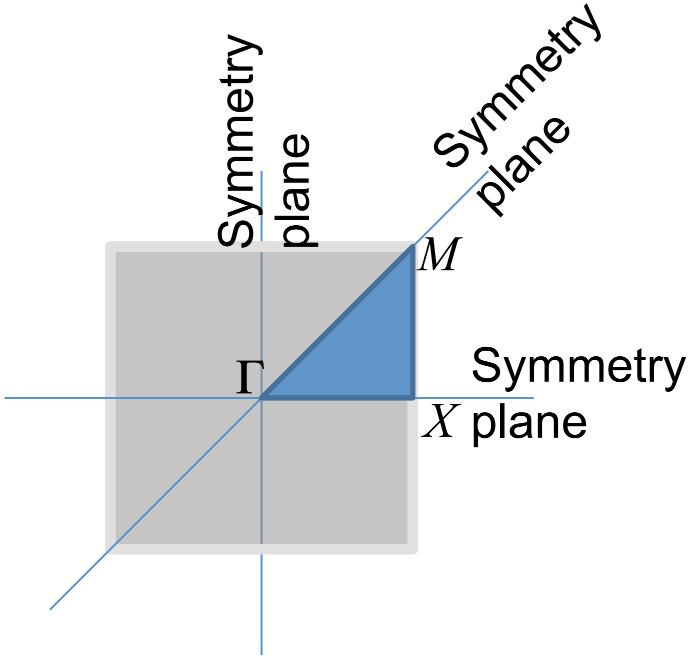
Reciprocal lattice of primitive vectors

$$\begin{cases} \vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1.(\vec{a}_2 \times \vec{a}_3)} = 2\pi \dfrac{a\vec{e}_2 \times \vec{e}_3}{a\vec{e}_1.(a\vec{e}_2 \times \vec{e}_3)} = 2\pi \dfrac{a\vec{e}_1}{a\vec{e}_1.(a\vec{e}_1)} = \dfrac{2\pi}{a}\vec{e}_1 \\ \vec{b}_2 = 2\pi \dfrac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_2.(\vec{a}_3 \times \vec{a}_1)} = \dfrac{2\pi}{a}\vec{e}_2 \\ \vec{b}_3 = \vec{e}_3 \end{cases}$$

Vectors of the reciprocal lattice

$$\vec{G} = m\vec{b}_1 + n\vec{b}_2 = \frac{2\pi}{a}\left(m\vec{e}_1 + n\vec{e}_2\right) = \frac{2\pi}{a}\vec{g},\ (m,n)\,\text{integers}$$

One shows that the first Brillouin zone is a square and due to the symmetries of this square, study can be limited to the triangle ΓXM ⇔ **Irreducible Brillouin zone *ΓXM***



$$\Gamma : \overrightarrow{\Gamma\Gamma} = \vec{0} \Rightarrow \Gamma : \frac{2\pi}{a}(0,0),$$

$$X : \overrightarrow{\Gamma X} = \frac{\vec{b}_1}{2} \Rightarrow X : \frac{2\pi}{a}\left(\frac{1}{2},0\right),$$

$$M : \overrightarrow{\Gamma M} = \frac{\vec{b}_1 + \vec{b}_2}{2} \Rightarrow M : \frac{2\pi}{a}\left(\frac{1}{2},\frac{1}{2}\right).$$

Γ, X, M : points of high symmetry

⇒*Calculation of the band structure for a wave vector*

$$\vec{K} = \frac{2\pi}{a}\vec{k} = \frac{2\pi}{a}\left(k_1\vec{e}_1 + k_2\vec{e}_2\right)$$

describing the periphery (ΓXM) of the irreducible Brillouin zone

Fourier transform of the equation of propagation for the Z modes

$$\omega^2 \sum_{G'} B^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{G'} A^{(33)}_{\vec{G},\vec{G}'} U_{3,\vec{K}}\left(\vec{G}'\right)$$

$$\omega^2 \sum_{G'} \rho\left(\vec{G}-\vec{G}'\right) U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{G'} C_{44}\left(\vec{G}-\vec{G}'\right)\left[\left(G_1+K_1\right)\left(G'_1+K_1\right)+\left(G'_2+K_2\right)\left(G_2+K_2\right)\right] U_{3,\vec{K}}\left(\vec{G}'\right)$$

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In the summations, one can separate the term $\vec{G}=\vec{G}'$ and one obtains

$$\omega^2\left\{\left[\rho(\vec{0})U_{3,\vec{K}}(\vec{G})\right]+\sum_{\vec{G}'\neq\vec{G}}\rho(\vec{G}-\vec{G}')U_{3,\vec{K}}(\vec{G}')\right\}=$$

$$=C_{44}(\vec{0})\left[(G_1+K_1)(G_1+K_1)+(G_2+K_2)(G_2+K_2)\right]U_{3,\vec{K}}(\vec{G})$$

$$+\sum_{\vec{G}'\neq\vec{G}'}C_{44}(\vec{G}-\vec{G}')\left[(G_1+K_1)(G'_1+K_1)+(G'_2+K_2)(G_2+K_2)\right]U_{3,\vec{K}}(\vec{G}')$$

$$\Leftrightarrow \omega^2\left\{\left[\overline{\rho}\,U_{3,\vec{K}}(\vec{G})\right]+(\rho_A-\rho_B).\sum_{\vec{G}'\neq\vec{G}}F(\vec{G}-\vec{G}')U_{3,\vec{K}}(\vec{G}')\right\}=$$

$$=\overline{C_{44}}(\vec{G}+\vec{K})^2U_{3,\vec{K}}(\vec{G})+(C_{44,A}-C_{44,B})\sum_{\vec{G}'\neq\vec{G}}F(\vec{G}-\vec{G}')\left[(\vec{G}+\vec{K})(\vec{G}'+\vec{K})\right]U_{3,\vec{K}}(\vec{G}')$$

$$\Leftrightarrow \omega^2\overline{\rho}\left\{U_{3,\vec{k}}(\vec{g})+\frac{(\rho_A-\rho_B)}{\overline{\rho}}.\sum_{\vec{g}'\neq\vec{g}}F(\vec{g}-\vec{g}')U_{3,\vec{k}}(\vec{g}')\right\}=$$

$$=\overline{C_{44}}\left(\frac{2\pi}{a}\right)^2\left\{(\vec{g}+\vec{k})^2U_{3,\vec{k}}(\vec{g})+\left(\frac{C_{44,A}-C_{44,B}}{\overline{C_{44}}}\right)\sum_{\vec{g}'\neq\vec{g}}F(\vec{g}-\vec{g}')\left[(\vec{g}+\vec{k})(\vec{g}'+\vec{k})\right]U_{3,\vec{k}}(\vec{g}')\right\}$$

$$\Leftrightarrow \Omega^2 \left\{ U_{3,\vec{k}}(\vec{g}) + (delp). \sum_{\vec{g}' \neq \vec{g}} F(\vec{g}-\vec{g}')U_{3,\vec{k}}(\vec{g}') \right\} =$$

$$= \left\{ \left(\vec{g}+\vec{k}\right)^2 U_{3,\vec{k}}(\vec{g}) + (delt). \sum_{\vec{g}' \neq \vec{g}} F(\vec{g}-\vec{g}') \left[\left(\vec{g}+\vec{k}\right)\left(\vec{g}'+\vec{k}\right)\right] U_{3,\vec{k}}(\vec{g}') \right\}$$

where $\Omega = \left(\dfrac{\omega}{\left(\frac{2\pi}{a}\right)\sqrt{\frac{\overline{C_{44}}}{\overline{\rho}}}} \right)$ $\quad delp = \dfrac{(\rho_A - \rho_B)}{\overline{\rho}}$ $\quad delt = \left(\dfrac{C_{44,A} - C_{44,B}}{\overline{C_{44}}} \right)$

In the course of the numerical resolution of this equation, we consider

integers m and n (components of the reduced reciprocal lattice vectors $\vec{g}$)

such as $-MT \le m \le +MT$ and $-MT \le n \le +MT$.

$(2MT+1)^2$ two-dimensional $\vec{g}$ vectors are taken into account.

This gives $(2MT+1)^2$ eigenfrequencies for a given wave vector.

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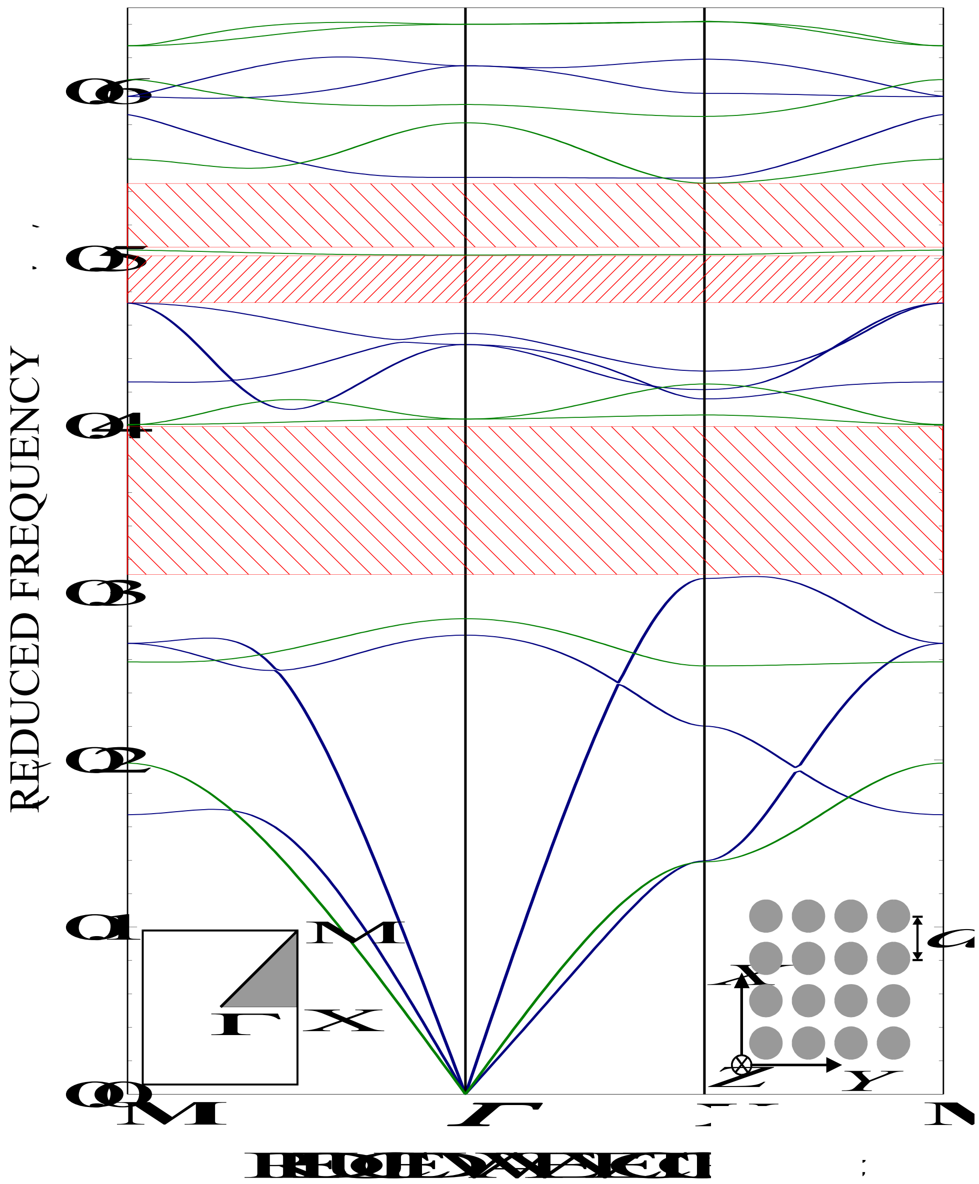
Example of MATLAB/OCTAVE code : Z_modes.m

Based on the code developed by Daniel Peter Elford
See "*Band gap formation in acoustically resonant phononic crystals*",
PhD thesis, Loughborough University, UK, November 2010,

https://dspace.lboro.ac.uk/2134/7071

Numerical implementation for the XY modes can be done in the same way but matrices are twice larger than those for the Z modes …

Example of band structure



Square array of Carbon cylinders

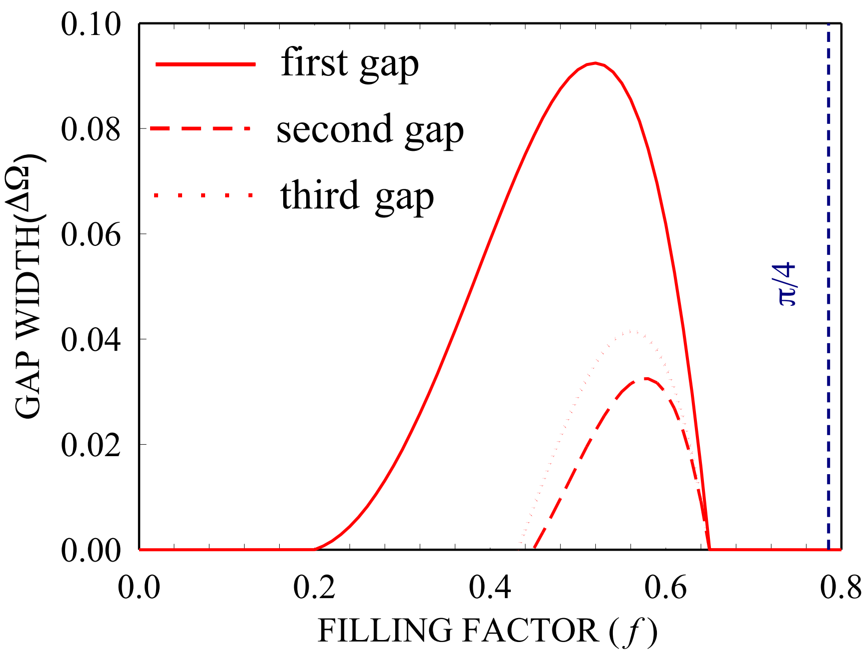
(circular cross section)

embedded in an epoxy resin matrix

***f* = 55 %**

Z modes

XY modes



Advantages and drawbacks of the PWE method

<u>Advantages</u> :

- Very easy to implement
- General (suitable *in theory* for 1D, 2D, 3D periodic structures)

<u>Drawbacks</u> :

- Convergence of the (truncated) Fourier series is slow especially for constituent materials with very different densities and moduli
- Not reliable for mixed solid/fluid structures except for
  - Rigid solid inclusions in air
  - Holes in a solid matrix

LOW CONVERGENCE OF THE FOURIER SERIES ?

Problem intensively studied for PWE method applied to photonic crystals at the begining of the 1990's

H.S. Sozuer *et al.*, Phys. Rev. B **45**, 13962 (1992)

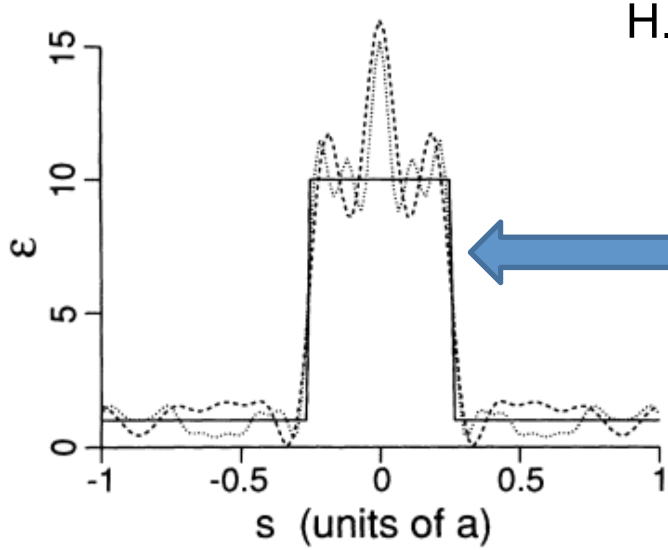


FIG. 2. $\epsilon(\mathbf{r})$ (solid) and $\epsilon_{trunc}(\mathbf{r})$ with N=331 (dashed) and N=1139 (dotted) for dielectric spheres in a fcc lattice along $x = y = z$ plotted against the path length s. $\epsilon_b = 1$, $\epsilon_a = 10$, and $\beta = 0.3$.

"It is clear that, just because increasing N does not produce visible differences in the resulting band structure, one has not necessarily converged to the "true" values. In this case, it is merely an indication of the slow convergence of the Fourier series."

In the Fourier transform, one replaces a strongly discontinuous function (density or elastic moduli) by a summation of continous sinusoïdal functions ….

Gibbs phenomenon

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PWE METHOD FOR MIXED SOLID/FLUID PHONONIC CRYSTALS ?

First case

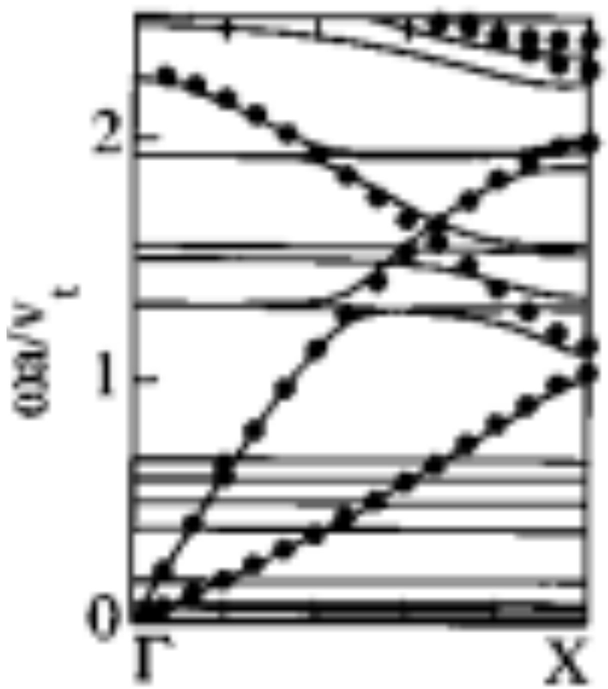
Square array of hollow cylinders in a solid matrix, filled with a non-viscous fluid

One may intuitively modelized the fluid as an isotropic *«solid»* material with C_{44}=0 because a transverse vibration does not exist inside a liquid …

… but the conventional PWE method still assumes a finite displacement amplitude for this transverse mode in the cylinders

⇒ numerical instabilities in the PWE code

Example:



XY modes in a two-dimensional square lattice of mercury circular cylinders in an Al matrix with filling fraction *f*=0.4.

Dots : FDTD method (“exact” method)

Lines : PWE method (with C_{44} for Hg ≡ 0)

⇒Fictitious flat bands

(number of these bands increases when number of $\vec{G}$ vectors taken into account in the Fourier series increases !!!)

Y. Tanaka *et al.,* Phys. Rev. B **62**, 7387 (2000)

Second case Square array of hollow cylinders (holes) in a solid matrix

Fluid inside the holes can not be treated as a solid medium with C_{44}=0 !!!!

For the same reason (fictitious flat branches), air inside the holes can not be replaced by vacuum with ρ=0 and $C_{11}=C_{44}$=0 !!!!

Low Impedance Medium (LIM) rather than vacuum

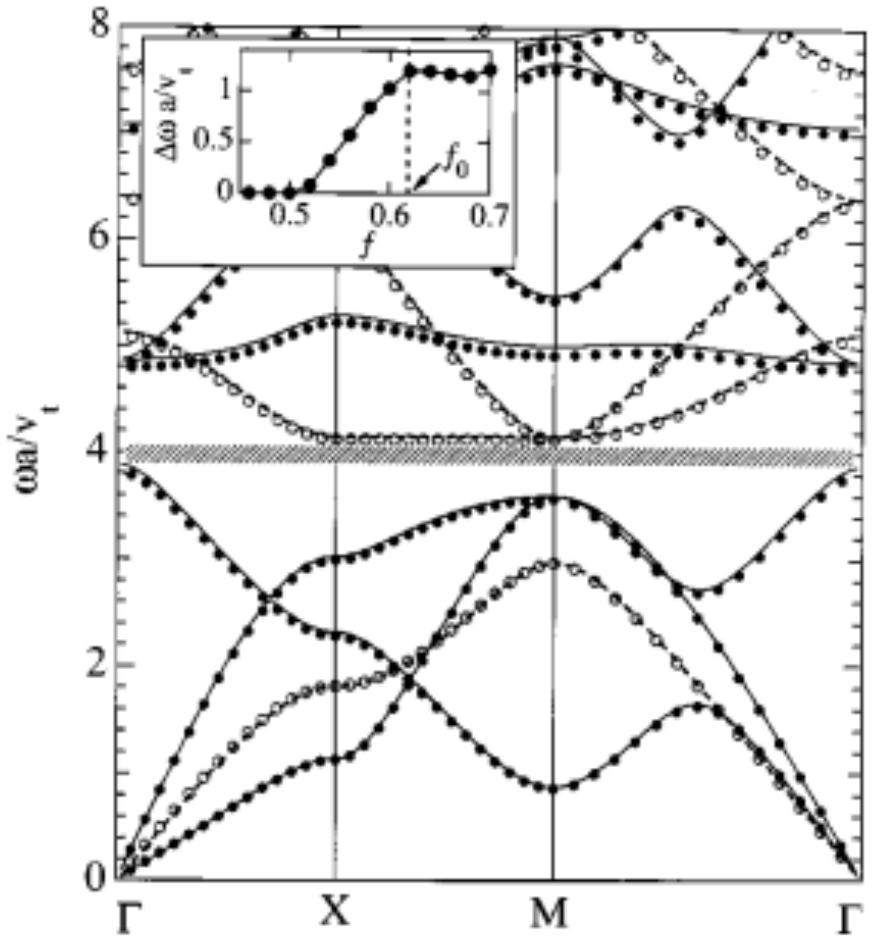
Low density $\cong 10^{-4}$ kg.m^{-3} (<< 10^{3} kg.m^{-3} for usual solids)

Low elastic moduli $\cong 10^{5}$ N.m^{-2} (<< 10^{10} N.m^{-2} for usual solids)

$\Rightarrow$ Low impedance $\cong$ 10 kg.m^{-2}.s^{-1} !!!

Example:

Y. Tanaka *et al.*, Phys. Rev. B **62**, 7387 (2000)
C. Goffeaux et al., Phys. Rev. B **64**, 075118 (2001)



XY modes in a two-dimensional square lattice of hollow cylinders in an Al matrix with filling fraction f=0.55.

Dots : FDTD method ("exact" method)

Lines : PWE method (with material inside the cylinders is the LIM)

⇒ Perfect agreement between FDTD and (PWE with LIM)

⇔ *Spurious flat branches expected to appear in the PWE calculation with "real" air inside the holes are pushed out to the very high-frequency region.*

Remark : With the LIM, the contrast between the physical characteristics of the solid matrix and those of the «inclusions» is lower (compared to air) and the convergence of the Fourier series is « faster »

Third case Square array of solid cylinders in air

* Due to the huge contrast between the physical characteristics of the solid and those of air, the solid cylinders are assumed infinitely hard (high density and high elastic moduli)

* It implies that the sound does not penetrate such inclusions, and hence the propagation of acoustic waves is predominant in air.

• Air is a fluid and only longitudinal waves can propagate in air

⇒ Equation of propagation of longitudinal acoustic waves in an inhomogeneous fluid medium

$$-\frac{\omega^2}{C_{11}(\vec{r})}p(\vec{r},t)=\vec{\nabla}.\left(\frac{1}{\rho(\vec{r})}\vec{\nabla}p(\vec{r},t)\right)$$

where $p(\vec{r},t) \equiv$ Acoustic pressure field

In a « periodic » fluid medium, the equation of propagation of acoustic waves can be Fourier transformed in the form

$$\omega^2 \sum_{G'} C_{11}^{-1}\left(\vec{G}-\vec{G}'\right) p_{\vec{K}}\left(\vec{G}'\right) = \sum_{G'} \rho^{-1}\left(\vec{G}-\vec{G}'\right)\left[\left(G_1+K_1\right)\left(G'_1+K_1\right)+\left(G'_2+K_2\right)\left(G_2+K_2\right)\right] p_{\vec{K}}\left(\vec{G}'\right)$$

Equation similar to that of Z modes in an infinite 2D solid/solid phononic crystal

$$\omega^2 \sum_{G'} \rho\left(\vec{G}-\vec{G}'\right) U_{3,\vec{K}}\left(\vec{G}'\right) = \sum_{G'} C_{44}\left(\vec{G}-\vec{G}'\right)\left[\left(G_1+K_1\right)\left(G'_1+K_1\right)+\left(G'_2+K_2\right)\left(G_2+K_2\right)\right] U_{3,\vec{K}}\left(\vec{G}'\right)$$

By analogy
$$\begin{cases} \text{Z modes} \leftrightarrow \text{Fluid} \\ \rho \leftrightarrow C_{11}^{-1} \\ C_{44} \leftrightarrow \rho^{-1} \end{cases}$$

$$C_{11} = \rho V_L^2$$

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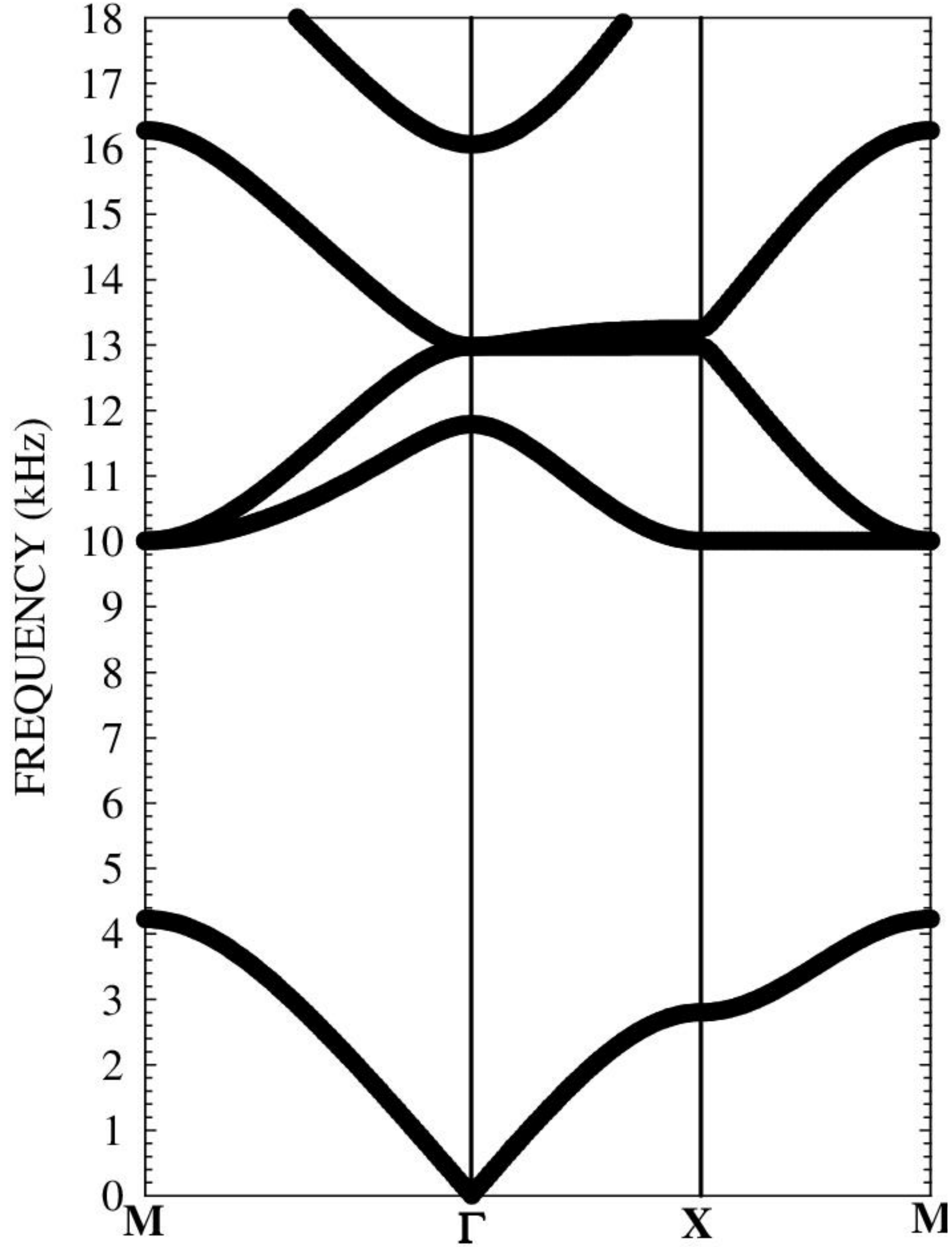
Example:

Square array of steel
cylinders in air
a = 2.7 cm
R= 1.29 cm

Stop band in the audible frequency range

↓

Sonic crystal



II) Extended PWE method for complex band structures, complex wave vectors, evanescent waves, examples.

"Classical" PWE expansion method $\Rightarrow$ For a fixed wave vector $\vec{K}$ (with real components), one calculates a set of real eigenfrequencies $\Omega_n\left(\vec{K}\right)$

"Extended" PWE expansion method $\Rightarrow$ For a fixed value of the frequency, one calculates the components of the wave vectors associated with the frequency

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Principle

In the classical PWE method, the Fourier transform of the equation of propagation of elastic waves in a phononic crystal leads to the resolution of a generalized eigenvalue equation in the form $\omega^2 \overleftrightarrow{B}.\vec{U} = \overleftrightarrow{A}.\vec{U}$.

The matrix elements of $\overleftrightarrow{A}$ involve terms depending on the components of the wave vector $\vec{K}$.

$\Rightarrow$ One may rewrite matrix $\overleftrightarrow{A}$ as $\overleftrightarrow{A} = K_\alpha^2 \overleftrightarrow{A}_1 + K_\alpha \overleftrightarrow{A}_2 + \overleftrightarrow{A}_3$ where K_α is one of the components of the wave vector and $\overleftrightarrow{A}_1$, $\overleftrightarrow{A}_2$ and $\overleftrightarrow{A}_3$ are matrices of the same size as $\overleftrightarrow{A}$. The generalized eigenvalue equation $\omega^2 \overleftrightarrow{B}.\vec{U} = \overleftrightarrow{A}.\vec{U}$ may be recast as $K_\alpha^2 \overleftrightarrow{A}_1.\vec{U} = \omega^2 \overleftrightarrow{B}.\vec{U} - \overleftrightarrow{A}_3.\vec{U} - K_\alpha \overleftrightarrow{A}_2.\vec{U}$ and can be rewritten as

$$K_\alpha \begin{pmatrix} \vec{\vec{I}} & \vec{\vec{0}} \\ \vec{\vec{0}} & \vec{\vec{A}}_1 \end{pmatrix} \begin{pmatrix} \vec{U} \\ K_\alpha \vec{U} \end{pmatrix} = \begin{pmatrix} \vec{\vec{0}} & \vec{\vec{I}} \\ \omega^2 \vec{\vec{B}} - \vec{\vec{A}}_3 & -\vec{\vec{A}}_2 \end{pmatrix} \begin{pmatrix} \vec{U} \\ K_\alpha \vec{U} \end{pmatrix} \text{ where } \vec{\vec{I}} \text{ is the identity matrix}$$

⇔ Eigen-value problem where the eigen-values are the component of the wave vector !

Example : Z elastic modes of a square array of cylinders of lattice parameter a embedded in a matrix

$$\omega^2 \sum_{G'} \rho(\vec{G}-\vec{G}') U_{3,\vec{K}}(\vec{G}') = \sum_{G'} C_{44}(\vec{G}-\vec{G}')\left[(G_1+K_1)(G'_1+K_1)+(G'_2+K_2)(G_2+K_2)\right] U_{3,\vec{K}}(\vec{G}')$$

Direction of propagation ΓX ⇒ $K_2=0$

$$K_1{}^2 \sum_{G'} C_{44}(\vec{G}-\vec{G}') U_{3,\vec{K}}(\vec{G}')$$
$$= \sum_{G'} \left\{\omega^2 \rho(\vec{G}-\vec{G}') - (G_1G'_1+G_2G'_2) C_{44}(\vec{G}-\vec{G}')\right\} U_{3,\vec{K}}(\vec{G}') - K_1 \sum_{G'} (G_1+G'_1) C_{44}(\vec{G}-\vec{G}') U_{3,\vec{K}}(\vec{G}')$$

and

$$K_1 \begin{pmatrix} \overleftrightarrow{I} & \overleftrightarrow{0} \\ \overleftrightarrow{0} & \overleftrightarrow{A}_1 \end{pmatrix} \begin{pmatrix} \vec{U} \\ K_1 \vec{U} \end{pmatrix} = \begin{pmatrix} \overleftrightarrow{0} & \overleftrightarrow{I} \\ \omega^2 \overleftrightarrow{B} - \overleftrightarrow{A}_3 & -\overleftrightarrow{A}_2 \end{pmatrix} \begin{pmatrix} \vec{U} \\ K_1 \vec{U} \end{pmatrix}$$

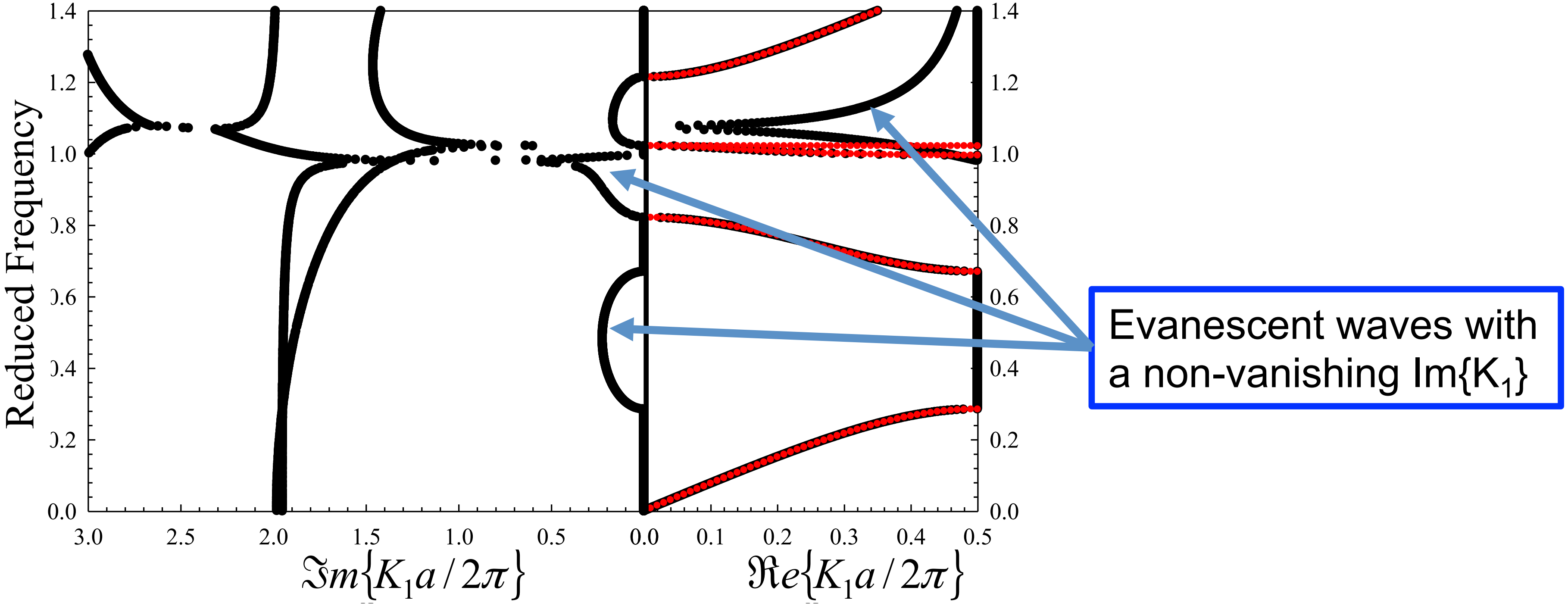
where

$$\left\{ \begin{aligned} B_{\vec{G},\vec{G}'} &= \rho\left(\vec{G}-\vec{G}'\right) \\ A^{(1)}_{\vec{G},\vec{G}'} &= C_{44}\left(\vec{G}-\vec{G}'\right) \\ A^{(2)}_{\vec{G},\vec{G}'} &= C_{44}\left(\vec{G}-\vec{G}'\right)\left(G_1 + G'_1\right) \\ A^{(3)}_{\vec{G},\vec{G}'} &= C_{44}\left(\vec{G}-\vec{G}'\right)\left(G_1 G'_1 + G_2 G'_2\right) \end{aligned} \right.$$

Eigen-value problem where, for a fixed value of the real frequency ω,

the complex eigen-values are $K_1 = \Re e\{K_1\} - i\Im m\{K_1\}$

An example of complex band structure

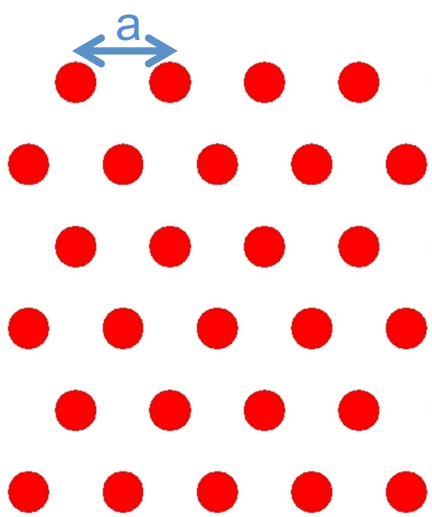


Band structure along the ΓX direction of the irreducible Brillouin zone for a square array of holes drilled in a Silicon matrix :

Red dots: Classical PWE method;
Black dots: Extended PWE method.

Steel-Epoxy phononic crystal

Triangular array of steel cylindrical inclusions embedded in an epoxy matrix
Inclusion radius : R=1mm
Lattice parameter : a=2.84 mm
$\Rightarrow$ Filling factor = 45%



Band structure

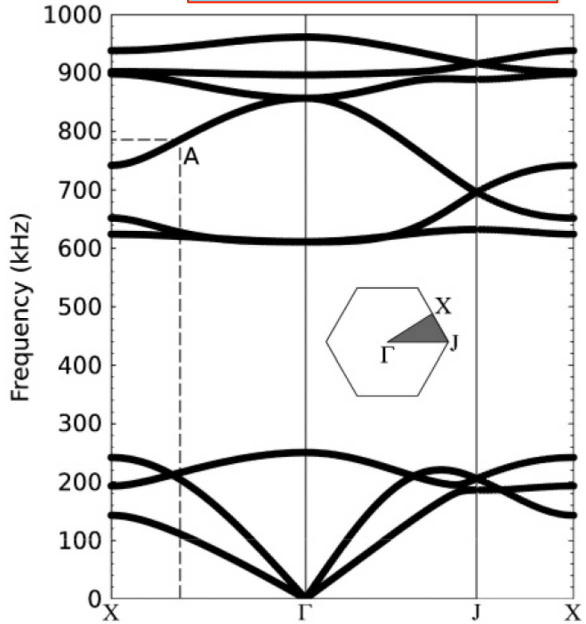


FIG. 1. Elastic band structure for the 2D PC made of a triangular array of steel rods in an epoxy matrix.

Equi-frequency contours
$(\omega = f(k_x,k_y))$

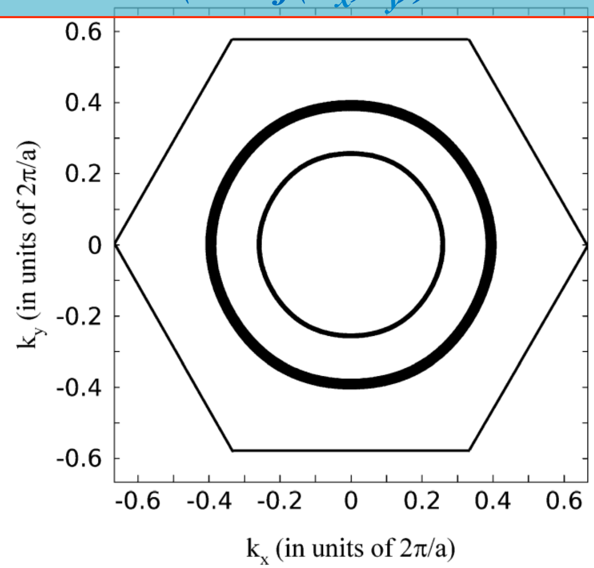


FIG. 3. EFCs of the PC at 780 kHz (thick line) and 820 kHz (thin line).

⇒ Refraction phenomena

CONCLUSION

The PWE method is a useful tool for calculating the band structures of phononic crystals but some limits (constituent materials solid or liquid, convergence …) restrict its use to some cases …