Calculation of band structures of a phononic crystal within a waveguide in 3D with cubic inclusions using a Periodic Green's Function Method

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Abstract. The Phononic Crystals have generated a growing scientific interest as a means to control the dispersion of waves in various technological applications such as telecommunications. In particular, Phononic Crystal Waveguides are composed of periodic distributions of dispersers immersed in a propagation medium and, designed by an arrangement with dimensions and periods comparable to the wavelength. These crystals have properties that give them the ability to guide acoustic waves efficiently. In this paper, we present a numerical Boundary Element Method, which requires the use of a Periodic Green's Function. This method allows to calculate the band structure of phononic crystals in two- and three-dimensions. In particular, the band structure is calculated for a waveguide formed by two flat, and parallel plates that involve a two-dimensional periodic arrangement of cubic inclusions. All surfaces involved are considered acoustic hard surfaces. The system considered, in addition to being a waveguide is in itself a phononic crystal, so that this type of systems present an alternative to manufacture to phononic crystal that can act as a phononic crystal and as an acoustic waveguide. These properties present some interest from a technological point of view.

1. Introduction

The Phononic Crystals (PnCs) are artificial structures composed of at least two materials with different mass density and elastic properties. These are constructed in such a way that the elastic constants and/or the mass density of this structured compound are periodic functions in space. The material type of the PnCs can be formed can be solid, liquid or gaseous. The PnCs are designed for the control of the propagation of acoustic waves. These allow covering a large part of the continuous sonic spectrum, from infrasound (hertz) to thermal waves (terahertz), passing through audible sounds (kilohertz), ultrasound (megahertz) and hipersound (gigahertz) [1].

The dimensions that intervene in the PnCs range from a few meters to a hundred nanometers. On this scale, matter appears as continuous, so that the laws of classical mechanics are applicable and are used as a general rule. PnCs open the possibility to develop novel materials with advantageous properties that arise from the ability to tailor the propagation of acoustic and elastic waves and with it its effective properties [2], so condensed matter physicists are beginning to take interest in them.

In literature, one can find a lot of works on PnCs; however, most of the works are limited to two-dimensional PnCs. So far, so both theoretically [2, 3] and experimentally [4, 5], only some examples of completely three-dimensional (3D) phononic crystals have been investigated. In most calculations the plane-wave expansion (PWE) method [6, 7] has been used. However, PWE method has shown to be inadequate for to produce accurate results for modeling periodic composites consisting of solid
spheres in a fluid host. Other techniques used to study acoustic problems are the finite-difference time-domain (FDTD) method [8], fast multipole boundary element method (FMBEM) [9] based on the Burton-Miller formulation, etc.

In particular, the Boundary Element Methods (BEMs) have been widely used to determine the scattered fields in two-dimensional (2D) and three-dimensional (3D) systems in optics, propagation of seismic waves, and acoustics [10, 11]. BEM has shown various advantages such as ease of coding and computational efficiency, so that has been proposed as a versatile method to determine the functions of the field and its normal derivative directly, in contrast to other methods that use the expansion of them into a functional basis [12]. It is possible that the most important feature of BEM is its versatility for solving resonant modes in cavities and scattering problems [13].

Among the possible applications of the PnC systems we can mention, of course, the acoustic isolation [14], the waveguides [15, 16] and another less intuitive is the use of these structures to focus the waves of the sea towards a plant with the purpose of converting mechanical energy into electrical energy [17].

In the present paper, we show a numerical study for a Phononic Crystal Waveguides (PnCWs) formed by 3D acoustic rectangular waveguides with internal structures, composed by an array of cubic inclusions periodically in two directions (3DPnCW). Surfaces considered are hard acoustic surfaces that correspond to Neumann boundary condition. This paper is organized as follows. Sec. 2 introduces a numerical integral method to try the physical system considered, based in the use of the Periodic Green's Function (PGF) method and BEM [18]. In Sec. 3, we show results of phononic band structures for a 3DPnCW with two different sizes of cubic inclusions. In this section, we also discuss the numerical results. Finally, we present our conclusions in Sec. 4.

2. Periodic Green's Function Method applied to calculation of the band structure of a phononic crystal within a waveguide in 3D with cubic inclusions

In this section, we will introduce a numerical method to calculate the band structure of a 3DPnCW formed by two flat plates that involve a periodic 2D array of cubic inclusions as shown in figure 1. It is considered that all surfaces involved are acoustic hard surfaces and the medium between the plates is air. The unit cell of the system is shown in figure 2.

Figure 1. Graphic description of a 3DPnCW formed by two flat and parallel acoustic surfaces that have a periodic arrangement of cubic inclusions.

Figure 2. Unit cell of a 3DPnCW formed by two flat and parallel surfaces that enclose a cubic inclusion.
For a linear acoustic pressure wave in each unit cell $P_{m,l}(r,t)$, in the time-harmonic case with frequency $\omega(P_{m,l}(r,t)=P_{m,l}(r)e^{i\omega t})$, the Helmholtz equation is satisfied and given by

$$\nabla^2P_{lm}(r) + \left(\frac{\omega}{c}\right)^2P_{lm}(r) = 0 \quad (1)$$

where $l, m \in \mathbb{Z}$, $c$ is the longitudinal speed of the wave in the acoustic medium and $r$ is the observer's position. The subscripts $l$ and $m$ represent the position of a cell in the direction $x$ and $y$ within the arrangement with two-dimensional periodicity, respectively. Our problem is to calculate the band structure of a periodic system, for this we propose to use an integral numerical method that can be formulated from a PGF and BEM to solve the equation of Helmholtz under Neumann boundary conditions (acoustic hard surfaces).

Periodicity in the $x$ and $y$-direction of the 3DPnCW is considered, thus the Bloch theorem can be applied. This implies the following four relations of periodicity:

$$P_{lm}(x + la,y,z,t) = e^{ik_xat}P_{0,m}(x,y,z) \quad (2)$$

$$P_{lm}(x,y + la,z,t) = e^{ik_yat}P_{l,0}(x,y,z) \quad (3)$$

$$\frac{\partial P_{lm}(x+la,y,z,t)}{\partial n} = e^{ik_xat}\frac{\partial P_{0,m}(x,y,z)}{\partial n} \quad (4)$$

and

$$\frac{\partial P_{lm}(x,y+la,z,t)}{\partial n} = e^{ik_yat}\frac{\partial P_{l,0}(x,y,z)}{\partial n} \quad (5)$$

where $\mathbf{k} = (k_x, k_y)$ is the two-dimensional Bloch vector.

In order to determine the band structure, the dispersion relation must be calculated. To do this, let us consider a Green's function for the 3D geometry given by

$$G(r,r') = \frac{e^{i\omega |r-r'|}}{|r-r'|} \quad (6)$$

where $r$ and $r'$ are observation and integration points, respectively. The Green's function is a solution to

$$\nabla^2G(r,r') + \left(\frac{\omega}{c}\right)^2G(r,r') = -4\pi\delta(r-r') \quad (7)$$

Considering the geometry of the system shown in figure 1, and applying the three-dimensional Green's second identity for a pressure wave $P_{lm}(r)$ and the Green's function $G$ in the air region, we obtain the expression

$$\sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\frac{1}{4\pi} \int_{S_{lm}} \left[G(r,r') \frac{\partial P_{lm}(r')}{\partial n} - \frac{\partial G(r,r')}{\partial n} P_{lm}(r')\right] dS' = \theta(r)P_{0,0}(r) \quad (8)$$

being $\theta(r) = 1$ if $r$ is inside the unit cell with $l = 0$ and $m = 0$, and $\theta(r) = 0$ otherwise. $dS'$ is the element of area, $\mathbf{n}'$ is the outward normal vector to $S_{lm}$, and the observation point $r$ is infinitesimally separated from surface $S_{lm}$.

Let us consider a numerical version of left-hand side of equation (8) taking a sampling of small surfaces denoted by $\Delta S_{lm}^n$, on the corresponding integration surface $S_{lm}$, with $n = 1, 2, ..., N$, such that

$$\sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\frac{1}{4\pi} \int_{S_{lm}} \left[G(r,r') \frac{\partial P_{lm}(r')}{\partial n} - \frac{\partial G(r,r')}{\partial n} P_{lm}(r')\right] dS' \approx \sum_{n=1}^{N} Q_n \left[ \frac{1}{4\pi} \sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \int_{\Delta S_{lm}^n} e^{ik_xat+ik_yam}G(r,r')dS'\right]$$

$$- \sum_{n=1}^{N} P_n \left[ \frac{1}{4\pi} \sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \int_{\Delta S_{lm}^n} e^{ik_xat+ik_yam}\frac{\partial G(r,r')}{\partial n}dS'\right] \quad (9)$$
being \( p_n \) and \( q_n \) the numerical values of the pressure, \( P_{0,0}(r') \) and \( \partial P_{0,0}(r')/\partial n' \) its normal derivative, evaluated at the \( n \)-th central point, denoted by \( R_n \), of the small surface elements \( \Delta S_{lm}^n \), respectively. In this way, equation (9) can be represented numerically in terms of a homogeneous system of algebraic equations as

\[
\sum_{j=1}^{N} L_{ij}(k, \omega) Q_j - \sum_{j=1}^{N} N_{ij}(k, \omega) P_j = 0
\]  

(10)

The matrix elements \( L_{ij}(k, \omega) \) and \( N_{ij}(k, \omega) \), that depend of the Bloch vector \( k \) and the frequency \( \omega \), are given by

\[
L_{ij}(k, \omega) = \sum_{l=-N_L}^{N_L} \sum_{m=-N_L}^{N_L} e^{i(k_x a l + k_y a m)} l_{ij}^{lm}(\omega) 
\]  

(11)

and

\[
N_{ij}(k, \omega) = \sum_{l=-N_L}^{N_L} \sum_{m=-N_L}^{N_L} e^{i(k_x a l + k_y a m)} N_{ij}^{lm}(\omega) 
\]  

(12)

where \( N_L \) is the maximum value of the indices \( l \) and \( m \), numerically considered. This positive integer number represents a simple form to truncate the series, if \( N_L \) is large enough, almost accurate results are obtained. Information about how the numerical values of \( L_{ij}^{lm}(\omega) \) and \( N_{ij}^{lm}(\omega) \) are obtained as outlined in Ref. [13].

Acoustic hard surfaces for the system are considered in this work. So that the normal derivative of the acoustic pressure is zero (Neumann boundary condition) on all the surfaces. This leads to \( Q_n = 0 \) for \( n=1,2,...,N \), thereby obtaining the expression

\[
\sum_{j=1}^{N} N_{ij}(k, \omega) P_j = 0, \quad i = 1,2,3,...,N
\]  

(13)

Equation (13) constitute a linear system \( M(\omega)F(\omega) = 0 \) that has an associated representative matrix, \( M \), which depends on the Bloch vector \( k \) and the frequency \( \omega \). Since the equation system is homogeneous, a nontrivial solution can be obtained if the determinant of such matrix is zero. To determine the frequency \( \omega \), we define the function

\[
D(k, \omega) = \ln(|\det(M)|)
\]  

(14)

Numerically, this function presents local minima points that will give us the numerical dispersion relation \( \omega = \omega(k) \). In this way, the band structure of the 3DPhCW can be calculated.

The complexity of the system is enough to not allow us from obtaining analytical solutions. However, to validate the application of the PGF method to calculate of the band structure of a 3DPhCW, let us consider a limiting case that presents an analytical solutions. A simple 3D waveguide formed by two flat, parallel and acoustic hard surfaces (without inclusions) has the analytical dispersion relation

\[
\omega(k = (k_x, k_y)) = \frac{p}{2\pi} \sqrt{\left(k_x - \frac{2\pi}{l} \right)^2 + \left(k_y - \frac{2\pi}{m} \right)^2 + \left(\frac{\pi}{q} \right)^2} 
\]  

(14)

where \( l, m = 0, \pm 1, \pm 2, \pm 3, ... \); \( q = 0, 1, 2, 3, ..., \) and the Bloch vector \( k = (k_x, k_y) \) within the first Brillouin zone. In the band structure it is common to introduce dimensionless quantities, so our results will be expressed in terms of a reduced frequency given by \( \omega_r = P/2\pi \omega \) and a reduced Bloch vector given by \( k_r = P/2\pi k \).

A comparison between the analytical and the corresponding numerical results for a 3D waveguide with acoustic hard surfaces is shown in figure 3, where the distance between the flat surfaces of \( b = 2\pi \) was considered, and \( N_L = 15 \). Analytical results are illustrated by the blue dotted curves and numerical results by the red dotted curves. Figure 3 shows that the phononic band structures calculated by both methods are overlap, showing an excellent concordance.

The excellent agreement between both band structures that is shown in figure 3 gives reliability to PGM to obtain accurate numerical results for more complex systems.
Figure 3. Band structures of an infinite 3DPnCW with acoustic hard surfaces. The distance between the walls is $2\pi$. Analytical model (blue dotted curves) and 3DPGFM (red dotted curves) are compared.

3. Phononic Band Structures of a 3DPnCW

The numerical results shown in figure 3 allows us to now consider a waveguide formed by two flat, parallel and acoustic hard surfaces that have a two-dimensional arrangement of cubic inclusions as shown in figure 1. Figure 4 shows the unit cell when the separation between flat surfaces is $b = 2\pi$, $a = 2\pi$, and $N_L = 20$, for (a) $c = 0.1\pi$ and (b) $c = 0.5\pi$. In figure 4(c) and (d), the band structures are shown for each configuration, respectively.

Figure 4. Unit cells for a 3DPnCW with $a = 2\pi$, $b = 2\pi$, and $N_L = 20$ with sides of inclusions equal to (a) $c = 0.1\pi$ and (b) $c = 0.5\pi$. In (c) and (d) their calculated band structures are shown, respectively.
Comparing figures 3 and 4(a), we can see that the difference between the band structures is minimal, which is in accordance with the fact that a small inclusion size compared to the dimensions of \( a \) and \( b \) slightly modifies the band structure. In this case the quotient between \( a \) and \( c \) is 20. We cannot say the same between figures 3 and 4(b) where the same quotient is 5, which is directly reflected in the difference of the band structures.

On the other hand, the computation time required for the calculation of the band structures increases considerably as the value of \( N_L \) grows. This can be seen from equation (11) where the value of \( N_L \) is involved in two summations. With similar parameters to those used in the numerical results shown and for values of \( N_L = 20 \), the computation time is around 30,000 minutes. As future work, parallel programming will be considered, which can help to considerably reduce the computation time required and thus to consider larger inclusions in order to find band gaps in the band structure.

4. Conclusions
In this work the band structures of a 3DPnCW formed by two hard, flat and parallel acoustic hard surfaces that enclose a two-dimensional periodic arrangement of cubes formed also by acoustic hard surfaces. Analytical structures were compared with those calculated by the numerical method implemented. The numerical results agree with those predicted by the theory showing reliability to make calculations with inclusions within the waveguide. In addition, band structures were calculated for the 3DPnCW considering small cubic inclusions. This system considered in addition to being a waveguide is in itself a phononic crystal, so that presents an alternative to manufacture to phononic crystal that can acting as a phononic crystal and as an acoustic waveguide. These properties are of great interest from a technological point of view.

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