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Waves in periodic media: Fourier analysis shortcuts and physical insights, case of 2D phononic crystals

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Abstract. Phononic crystal is a structured media with periodic modulation of its physical properties that influences the propagation of elastic waves and leads to a peculiar behaviour, for instance the phononic band gap effect by which elastic waves cannot propagate in certain frequency ranges. The formulation of the problem leads to a second order partial differential equation with periodic coefficients; different methods exist to determine the structure of the eigenmodes propagating in the material, both in the real or Fourier domain. Brillouin explains the periodicity of the band structure as a direct result of the discretization of the crystal in the real domain. Extending the Brillouin vision, we introduce digital signal processing tools developed in the frame of distribution functions theory. These tools associate physical meaning to mathematical expressions and reveal the correspondence between real and Fourier domains whatever is the physical domain under consideration. We present an illustrative practical example concerning two dimensions phononic crystals and highlight the appreciable shortcuts brought by the method and the benefits for physical interpretation.

1. Introduction

Man-made periodic media have emerged several decades ago [1, 2] and have drawn much attention: they offer a mean to control the propagation of waves; yet one dimension photonic periodic structures like fibre Bragg gratings, multilayer dielectric mirrors or Distributed Feed-Back laser have reached industrial maturity and allow the effective control of photons. Such devices for phonon would be highly desirable; in fact, any kind of wave could be subject to such practical developments: the existence of band structures in Fourier domain is a universal feature of media periodicity regardless the nature of propagating wave. Wave propagation in periodic media is governed by a second order partial differential equation with periodic coefficients. Usually, the general form of the solutions, the so called Bloch modes, are determined either in the real (direct) domain or in the Fourier (reciprocal) domain. Brillouin has exploited the two domain correspondence in order to explain the behaviour of the band structure [3]. In this paper we go on with the Brillouin conception of the direct and reciprocal domains correspondence, we derive an expression of the Bloch theorem in the Fourier domain. Along the way we show that the general form of the solutions (Bloch modes) comes out naturally as a consequence of media periodicity. The cornerstone of the proposed method is to introduce the Dirac delta comb to express the periodic media parameters in the equation system. The property of Dirac delta comb have been extensively studied in the frame of distribution functions theory and are well known, we take advantage of namely: the replicating property, the shifting property and the sifting



property along with their associated Fourier transform properties. These properties are intensively used in digital signal processing; the reader who isn't familiar with these notions can find a detailed summary in [4] that gives a survey of classical methods to establish wave properties in periodic media. In section two, we present the proposed method and show how straightforward it is to establish the wave equation for elastic waves in two-dimension periodic media and Dirac comb properties are briefly recalled. Then, in section three, we highlight the benefits of the proposed method for physical interpretation. We end up with some concluding remarks.

2. Elastic waves in 2D periodic media

In this section, we establish the expression of periodic media parameters as a function of a Dirac comb in direct domain and we derive the expression of the reciprocal domain wave equation.

2.1. Expression of the elastic wave equation in direct and reciprocal domains

Starting from the dynamic equation of motion for the displacements u_i and the expression of the stress tensor σ_{ij} , the well-known acoustic wave equation in a homogeneous media is:

$$\rho(\mathbf{r}) \frac{\partial^2 u_i(\mathbf{r})}{\partial t^2} = \sum_j \left(\frac{\partial}{\partial x_j} \left[\sum_{kl} c_{ijkl}(\mathbf{r}) \frac{\partial u_k(\mathbf{r})}{\partial x_l} \right] \right) \quad (1)$$

With $\rho(\mathbf{r})$ the mass density and $c_{ijkl}(\mathbf{r})$ the stiffness tensor of the considered media.

Assuming an harmonic dependence of the form $e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})}$ and recalling that a simple product in real domain converts to a convolution product (represented by \otimes) in reciprocal domain, the Fourier transform of the wave equation (1) writes :

$$\rho(\mathbf{k}) \otimes (-\omega^2 u_i(\mathbf{k})) = \sum_j \left(-ik_j \left[\sum_{kl} c_{ijkl}(\mathbf{k}) \otimes (-ik_l u_k(\mathbf{k})) \right] \right) \quad (2)$$

Now consider the shifting property that reads: $u(\mathbf{r}) \otimes \delta(\mathbf{r} - \mathbf{R}) = u(\mathbf{r} - \mathbf{R})$ and let $o(\mathbf{r})$ be the restriction of the mass density of a periodic media to one period. Thus, thanks to the replicating property, $\rho(\mathbf{r})$ and its Fourier transform can be expressed as:

$$\rho(\mathbf{r}) = o(\mathbf{r}) \otimes \sum_{\mathbf{R} \in R} \delta(\mathbf{r} - \mathbf{R}) \quad \Leftrightarrow \quad \rho(\mathbf{k}) = o(\mathbf{k}) V_{RL} \sum_{\mathbf{G} \in G} \delta(\mathbf{k} - \mathbf{G}) \quad (3)$$

where R and G are the direct and reciprocal lattices, V_{RL} stands for the reciprocal lattice unit cell volume and the symbol \Leftrightarrow stands for the Fourier transform operation. Hereafter, we refer to this kind of formulations as the Real (or Fourier) Domain Close Form Expression: RD-CFE (FD-CFE). Similar expressions can be written for $c_{ijkl}(\mathbf{r})$ the stiffness tensor defining $\gamma_{ijkl}(\mathbf{r})$ as its restriction to a period. Substituting the FD-CFE for mass density and stiffness tensor in equation (2), the Fourier domain wave equation becomes:

$$\begin{aligned} & \left(\sum_{\mathbf{G}} o(\mathbf{G}) \delta(\mathbf{k} - \mathbf{G}) \right) \otimes (-\omega^2 u_i(\mathbf{k})) \\ &= \sum_j \left((-ik_j) \left[\sum_{kl} \left(\sum_{\mathbf{G}} \gamma_{ijkl}(\mathbf{G}) \delta(\mathbf{k} - \mathbf{G}) \right) \otimes (-ik_l u_k(\mathbf{k})) \right] \right) \end{aligned} \quad (4)$$

We recall that the convolution product with a Dirac comb shifts the functions so that equation (4) gives us:

$$\omega^2 \left(\sum_{\mathbf{G}} o(\mathbf{G}) u_i(\mathbf{k} - \mathbf{G}) \right) = \sum_j \left(k_j \left[\sum_{kl} \sum_{\mathbf{G}} \gamma_{ijkl}(\mathbf{G}) (k_l - G_l) u_k(\mathbf{k} - \mathbf{G}) \right] \right) \quad (5)$$

Equation (5) is the Fourier domain expression of the elastic wave equation. In the above development, since no assumption was made concerning the nature of the solution, the variable \mathbf{k} is considered as continuous (not discrete).

2.2. Case of a transverse elastic wave in a two dimension lattice

To avoid the unnecessary heaviness of the tensor product in equation (5) in the discussion that follows and without loss of generality about the method presented, we restrict this section to the 2-D periodic media. Moreover, we limit ourselves to a special case where the coupling between the longitudinal and transversal waves does no longer exist. This situation appears in all crystal symmetries excluding trigonal and triclinic. More specifically, we consider a media with 2D periodicity in the (x, y) plane and uniformity along the z direction where a transverse acoustic wave propagates in the (x, y) plane with a displacement polarised along the z axis. In this situation equation (5) leads to scalar wavefunctions and writes:

$$\omega^2 \left(\sum_{\mathbf{G}} o(\mathbf{G}) u_3(\mathbf{k} - \mathbf{G}) \right) = k_1 \left[\sum_l \sum_{\mathbf{G}} \gamma_{313l}(\mathbf{G}) (k_l - G_l) u_3(\mathbf{k} - \mathbf{G}) \right] + k_2 \left[\sum_l \sum_{\mathbf{G}} \gamma_{323l}(\mathbf{G}) (k_l - G_l) u_3(\mathbf{k} - \mathbf{G}) \right] \quad (6)$$

Introducing Voigt notation, we substitute the fourth rank tensor expression of the unit cell elastic constants by the equivalence: $\gamma_{31kl} = \gamma_{5m}$; $\gamma_{32kl} = \gamma_{4m}$. Again, for the sake of simplicity we further exclude monoclinic crystals thus: $\gamma_{55} = \gamma_{44}$; $\gamma_{45} = \gamma_{54} = 0$ and equation (6) reduces to:

$$\omega^2 \left(\sum_{\mathbf{G}} o(\mathbf{G}) u_3(\mathbf{k} - \mathbf{G}) \right) = \sum_{\mathbf{G}} \gamma_{44}(\mathbf{G}) \mathbf{k} \cdot (\mathbf{k} - \mathbf{G}) u_3(\mathbf{k} - \mathbf{G}) \quad (7)$$

2.3. Correspondence with traditional methods

Equation (7) is the Fourier domain expression of the transverse elastic wave equation in a 2D periodic media; we have implicitly assumed a harmonic dependence of the wave in the form of $e^{-i\mathbf{k} \cdot \mathbf{r}}$. The correspondence with traditional methods which suppose as a starting point that the solutions are Bloch functions (i.e. a superposition of harmonics of the form $e^{-i(\mathbf{k} + \mathbf{G}'') \cdot \mathbf{r}}$ [5]) is simply found by substituting \mathbf{k} by $\mathbf{k} + \mathbf{G}''$ and changing the dummy variable \mathbf{G} to $\mathbf{G}' = \mathbf{G}'' - \mathbf{G}$ in (7).

3. The two domain correspondence

We discuss how the proposed method is a helpful tool for physical insights in the domain of wave propagation in periodic media.

3.1. Physical content of the formalism

In this section, we show how the periodicity of the band structure in Fourier domain as well as the general expression of Bloch functions are implicit results of equation (7).

3.1.1. Periodicity of the band structure in Fourier domain. A close inspection of equation (7) reveals that when we consider a fixed wave vector \mathbf{k} , we are in fact handling a subsystem of coupled linear equations that contains all shifted values of \mathbf{k} by reciprocal lattice vectors, as expressed by the sum over all reciprocal vectors $\mathbf{G} \in G$. This justifies the periodicity of the band structure in Fourier domain since any $\mathbf{k}' = \mathbf{k} + n\mathbf{G}$ leads to the same subsystem (permutation of its rows) with the same solutions. Also this observation justifies the restriction of \mathbf{k} over its principal values i.e. the first Brillouin zone.

3.1.2. Bloch theorem as a consequence of band structure periodicity. Having established the periodicity of the band structure, it appears that if we consider a travelling mode with a fixed eigen-frequency ω . It will contain all the discrete Fourier components of the form $\mathbf{k}_0 = \mathbf{k} - \mathbf{G}$. We can write:

$$u_{3,\mathbf{k}_0}(\mathbf{k}) = \sum_{\mathbf{G} \in G} u_3(\mathbf{k}_0 - \mathbf{G}) \delta(\mathbf{k} - (\mathbf{k}_0 - \mathbf{G})) \quad (8)$$

The inverse Fourier transform of equation (8) gives us:

$$u_{3,\mathbf{k}_0}(\mathbf{r}) = \frac{1}{2\pi} \left(\sum_{\mathbf{G} \in G} u_3(\mathbf{k}_0 - \mathbf{G}) e^{i\mathbf{G}\mathbf{r}} \right) e^{-i\mathbf{k}_0\mathbf{r}} \quad (9)$$

The term between parentheses is a periodic function in real domain; we recognise the general expression of Bloch function. So Bloch theorem comes out naturally as a consequence of media periodicity, our unique assumption. Indeed, in equation (7) we consider the Fourier transform $u_3(\mathbf{k})$ of the wavefunction as a continuous function of \mathbf{k} (and not a discrete one). Consequently, we have not anticipated any assumption concerning the wavefunction periodicity. It is the discrete nature of the periodic media parameters Fourier components $\rho(\mathbf{k})$ as expressed by expression (3) as well as $c_{ijkl}(\mathbf{k})$ that introduce the summation term over the reciprocal lattice vectors in equation (7). As mentioned above this term generates a selective coupling of such Fourier components whose wavevectors are of the form $(\mathbf{k}' = \mathbf{k} - \mathbf{G})$. In turn, this selective coupling explains why the initial "infinite equation system" splits into an infinite set of "infinite but numerable subsystems" each of these subsystems belongs to a fixed \mathbf{k} -value in the first Brillouin zone. Finally, the discretization of the Fourier components of $u_3(\mathbf{k})$ is a consequence of the summation term in equation (7). We recall that this summation term has been introduced by the convolution product with $\rho(\mathbf{k})$ and $c_{ijkl}(\mathbf{k})$ which are weighted Dirac combs.

3.2. Comments

We have presented a formalism that is devoted to derive the Fourier domain mathematical expression of wave equations in periodic media. This approach takes full advantage of digital signal processing techniques specifically, the replicating property i.e. the convolution with Dirac combs. Its derivation within the framework of distribution functions theory enables one to express the periodic coefficients in terms of continuous Fourier transform rather than Fourier series. This seemingly minor point appears to be crucial. On the one hand, the mathematical tools closely match the periodic media both in the real and the Fourier domains [4]. On the other hand, it leads to appreciable shortcuts: the problem reduces to a two steps procedure: having established RD and FD-CFE of the periodic coefficients, the Fourier domain formulation of the wave equation may be written by simple inspection.

Finally, we have illustrated the clearness and the straightforwardness of the formalism using the practical case of elastic waves in 2D periodic media. These features are direct results respectively of: First, from a conceptual point of view, thanks to the replicating property, the method clearly dissociates the contribution of the lattice as depicted by the Dirac comb from the contribution of the unit cell as depicted by the restriction of the physical parameters. Second, from a mathematical point of view, the concept of reciprocal lattice and its correspondence with the direct lattice is an already solved problem in the field of distribution functions theory as emphasized by the Fourier transform pair RD-CFE \Leftrightarrow FD-CFE.

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