Universality and optimality of band-gaps in laminated media

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We find that the frequency spectra of layered phononic and photonic composites admit a universal structure, independent of the geometry of the periodic-cell and the specific physical properties. We show that this representation extends to highly deformable and multi-physical materials of tunable spectra. The structure is employed to establish universal properties of the corresponding band-gaps, and to rigorously determine their statistical and optimal characteristics. Specifically, we investigate the density of the gaps, their maximal width and expected value. As a result, rules for tailoring the laminate according to desired spectra properties follow. Our representation further facilitates characterizing the tunability of the band-structure of soft and multi-physical materials.

Wave propagation in heterogeneous media has fascinated the scientific community for decades. The inhomogeneity causes multiple scattering, and, in turn, wave interferences that give rise to intriguing phenomena in various fields. Of particular interest are the transition of conducting to isolating behavior of electronic crystals [1], localization of electromagnetic waves in dielectrics [2], and attenuation of mechanical motions [3–8] in elastic media. The significance of the latter stems from its central role in numerous applications; transducers [9], waveguides [10], vibration filters [11], acoustic imaging for medical ultrasound and nondestructive testing [12], noise reduction [13] and cloaking [14, 15] are just a few examples. The mathematical and physical richness of elastic waves in heterogeneous materials emanates from their vectorial nature, and their spatial dependency on additional constituents parameters.

Layered media have been extensively studied [16–22], in virtue of their relative simplicity of fabrication and theoretical modeling. This letter provides new insights on the relation between their geometry, physical properties, and frequency spectrum. We find a universal representation for the spectrum, independent of the unit-cell geometry and specific constituents properties. This structure reveals a universal property of the gaps-density, namely, its invariance under the change of various geometric and physical properties. We utilize this representation to determine exactly the density of the gaps, and their expected and maximal widths. These results are identified with classes of compositions, hence provide rules for tailoring the laminate according to desired spectra characteristics. Thus far, such calculations would necessitate the truncation of infinite spectra, thereby leading to estimates rather than accurate results.

The canvas upon which the analysis is presented is of phononic crystals. The conclusions we draw, however, extend to additional systems. In virtue of the similarity between electromagnetic and elastodynamics wave equations for the considered geometry, our insights apply to one-dimensional (1D) photonic crystals as well. Stratified piezoelectrics admit a similar spectrum too [23]. Our analysis further applies to soft non-linear media and multi-physical composites, whose physical properties are changed upon application of external stimuli. By these means, the frequency spectrum of such materials is rendered tunable. Our approach facilitates characterizing this tunability, as demonstrated in the forthcoming.

We begin by considering a 1D crystal made out of two alternating phases (Fig. 1a). We denote the phases with 1 and 2, and their associated quantities with superscript (p), p = 1 and 2, respectively. The dispersion relation governing the propagation of waves in the crystal is [16, 20, 24]

\[
\arccos \eta = k_B h, \tag{1}
\]

where

\[
\eta = \cos \frac{\omega h^{(1)}}{c^{(1)}} \cos \frac{\omega h^{(2)}}{c^{(2)}} - \gamma \sin \frac{\omega h^{(1)}}{c^{(1)}} \sin \frac{\omega h^{(2)}}{c^{(2)}}. \tag{2}
\]

In the above, $\omega$ is the frequency, $k_B$ is the Bloch-parameter, $h^{(p)}$ is the thickness, and $h = h^{(1)} + h^{(2)}$. The parameter $c^{(p)}$ corresponds to different velocities, depending on the type of media and waves considered. Specifically, when the crystal is phononic, $c^{(p)}$ is the velocity of light in the phase; when the crystal is phononic, $c^{(p)}$ is the velocity of either transverse waves or longitudinal waves, propagating in a bulk. The parameter $\gamma = \frac{1}{2} (\alpha c^{(1)} / c^{(2)} + \alpha^{-1} c^{(2)} / c^{(1)})$ quantifies the contrast between the constituents impedance, where $\alpha = 1$ in the photonic case, and $\alpha = \rho^{(1)} / \rho^{(2)}$ in the phononic case, $\rho^{(p)}$ being the mass density. The frequency spectrum is obtained by solving Eq. (1) for values of $k_B$ in the irreducible 1st Brillouin zone [25], $0 \leq k_B h \leq \pi$. Band-gaps correspond to
ranges of frequencies of attenuating waves, for which $|\eta| > 1$ (Fig. 1b).

Our analysis of the spectrum benefits from a technique developed for the study of Schrödinger operators on metric graphs [26–28]. The systems we consider necessitate a suitable variation of that approach, as follows. Upon defining the variables

$$\zeta(p) := \frac{\omega h(p)}{c(p)},$$  \hspace{1cm} (3)

one can write $\eta$ as a doubly $2\pi$-periodic function of $\zeta^{(1)}$ and $\zeta^{(2)}$, namely

$$\eta \left( \zeta^{(1)}, \zeta^{(2)}; \gamma \right) := \cos \zeta^{(1)} \cos \zeta^{(2)} - \gamma \sin \zeta^{(1)} \sin \zeta^{(2)}.$$  \hspace{1cm} (4)

Fixing $\gamma$, we consider $\eta$ as a function defined on a 2D torus of edge length $2\pi$, characterized by the coordinates $\{\zeta^{(1)}, \zeta^{(2)}\}$. The absolute value $|\eta|$ is invariant under the transformations $\zeta^{(p)} \to \zeta^{(p)} + \pi$. This symmetry allows to make a further reduction, and fold the torus into a $\pi$-periodic torus; we denote the new torus by $T$, and denote by $D$ its subdomain where $|\eta| > 1$, i.e., where Eq. (1) is solved with imaginary $k_B$. For illustration, representative contours of the dispersion relation of real $k_B$ are plotted in Fig. 2a, on the unfolded torus, at $\gamma = 5$. Also, representative domains of $D$, at exemplary values of $\gamma = 2, 5$ and 10, are depicted in Fig. 2b, by the gray, blue, and red regions, respectively.

This geometric representation engenders new insights on universal characteristics of the frequency spectrum, as shown in the sequel. Towards this end, we interpret Eq. (3) as one which defines the following flow on $T$

$$\zeta'(\omega) = \omega \cdot \left( \frac{h^{(1)}}{c^{(1)}}, \frac{h^{(2)}}{c^{(2)}} \right) \mod \pi,$$  \hspace{1cm} (5)

where $\omega$ has the role of a time-like parameter. Band-gaps are identified with values of $\omega$ for which the flow $\zeta'(\omega)$ coincides with $D$. We denote the lower and upper curves bounding $D$ by $C_l$ and $C_u$, respectively. We find that $\eta = -1$ on these curves [29]; plugging this value into Eq. (4) provides the following expressions for the curves

$$\zeta^{(2)} = \pi - \arccos \left[ \frac{\cos \zeta^{(1)} \pm \gamma \sqrt{\gamma^2 - 1} \sin^2 \zeta^{(1)}}{1 + (\gamma^2 - 1) \sin^2 \zeta^{(1)}} \right],$$  \hspace{1cm} (6)

where the upper (resp. lower) curve $C_u$ (resp. $C_l$), corresponds to the plus (resp. minus) sign in the numerator. The function $\eta$ on $T$ is invariant under $\pi$-rotation of $T$ around its middle, given by the transformation $(\zeta^{(1)}, \zeta^{(2)}) \to (\pi - \zeta^{(1)}, \pi - \zeta^{(2)})$, and under reflection across the line $\zeta^{(2)} = \pi - \zeta^{(1)}$, by the transformation $(\zeta^{(1)}, \zeta^{(2)}) \to (\pi - \zeta^{(2)}, \pi - \zeta^{(1)})$. Each of those transformations leaves the domain $D$ invariant and exchanges between its boundary curves $C_l$ and $C_u$.

The direction of the flow on the torus is given by the ratio

$$a = \frac{\dot{h}^{(2)}}{\dot{h}^{(1)}} \frac{c^{(1)}}{c^{(2)}}.$$  \hspace{1cm} (7)

The irrationality of the ratio, on account of the physical nature of the parameters involved, implies that the flow covers the torus ergodically, with a uniform measure. Hence, the density of the gaps is simply the relative area of $D$ in $T$, which can be calculated via the integral of the closed-form expression

$$1 - 2 \frac{\pi}{\pi} \int_0^\pi C_l d\zeta^{(1)}.$$  \hspace{1cm} (8)

We arrive at a counter-intuitive and peculiar result; at a prescribed $\gamma$, the gap-density is independent of the volume fractions of the phases. To shed light on the significance of this statement, consider the following example. Compose a laminate of equal volume fractions of materials (1) and (2). Composite a second laminate by introducing an infinitesimal amount of (1) into a bulk of (2). The probability that an arbitrary frequency pertains to a band-gap is identical in the two laminates.

The widths of the gaps are investigated next. We recognize that these widths, which we denote by $\Delta \omega$, are related to lengths of intervals directed along the flow, which we denote by $\Delta \zeta$, whose endpoints lie on $C_u$ and $C_l$, via

$$\Delta \omega = \Delta \zeta \frac{\kappa^{(1)}}{\sqrt{1 + a^2}},$$  \hspace{1cm} (9)

where $\kappa^{(p)} = c^{(p)}/h^{(p)}$. We associate each length $\Delta \zeta$ with the parameters $a$ and $b$ which characterize the line equation of its corresponding flow interval

$$\zeta^{(2)} = a \zeta^{(1)} + b.$$  \hspace{1cm} (10)

These observations, together with the derived expressions for the curves $C_u$ and $C_l$, enable determining the width of the gaps, and relating it to the physical and geometrical properties of the crystal. As the whole spectrum is encapsulated in the torus, we are able, in turn, to formulate optimization problems rigorously, derived in the sequel.
We start with the 1st gap, whose width maximization is of practical importance, being the one which is most often realized experimentally [17, 20, 21]. We would like to know: given two materials, what is the microstructure which maximizes the 1st gap? The 1st gap is identified with the flow line emanating from the origin. Therefore, we seek the slope \( a \) which maximizes the right-hand side of Eq. (9), at \( b = 0 \). The problem is interpreted as a search for an optimal \( h^{(2)}/h^{(1)} \) at fixed \( \epsilon^{(p)} \).

To that end, the calculation over the torus serves as an alternative to a calculation of the 1st gap-width for all possible compositions, via a partial evaluation of the spectra. Calculations over the torus become a necessity, however, when the whole spectrum needs to be analyzed. Such cases are considered next, starting with the calculation of the greatest gap width. We address two different practical scenarios. The first scenario considers a given crystal, with prescribed geometrical and physical properties. The objective is delivered by finding the maximal \( \Delta \zeta \) within the segments along flows of the prescribed slope \( a \), i.e., maximizing over translations \( b \), and plugging it into Eq. (9). We emphasize that this optimization is defined solely over \( \mathbb{D} \), in an exact manner. Contrarily, a direct approach will require the evaluation of an infinite spectrum; since in practice it must be truncated, such approach provides only an approximation. The second scenario we consider is of a laminate with prescribed constituents, prior to determining their volume fractions. In this case, the maximal gap is obtained by maximizing the right-hand side of Eq. (9), over all slopes \( a \) and translations \( b \).

We supplement the discussion regarding optimality noting that our approach allows for quick calculation of bounds on the gaps-width, based on bounding \( \Delta \zeta \). We find that for \( \gamma < \gamma_{cr} \), where \( \gamma_{cr} \approx 5.45 \), the maximal \( \Delta \zeta \), denoted \( \Delta \zeta_{max} \), is obtained at the intersection of \( \mathbb{D} \) with \( \zeta^{(1)} = \pi/2 \). Utilizing Eq. (6), it is expressed in closed-form as

\[
\Delta \zeta_{max} = \pi - 2 \arccos \left( \frac{\sqrt{\gamma^2 - 1}}{\gamma} \right),
\]

(11)

When \( \gamma > \gamma_{cr} \), associated with large impedance contrast, \( \Delta \zeta_{max} \) is attained along the diagonal, for which \( \zeta^{(1)} = \zeta^{(2)} \). Upon substitution of \( \Delta \zeta_{max} \) into Eq. (9), the following bound is derived

\[
\Delta \omega < \frac{\kappa^{(1)} \kappa^{(2)}}{\sqrt{\left( \kappa^{(1)} \right)^2 + \left( \kappa^{(2)} \right)^2}} \Delta \zeta_{max}.
\]

(12)

Thus, an explicit expression in terms of the crystal properties is obtained. So far, to the best of our knowledge, such bounds were not accessible.

The analysis is concluded with expressions for statistical characteristics of the spectra, evaluated exactly using our representation. Specifically, the expected value of the gap-width of a prescribed system is determined via

\[
\frac{1}{\sqrt{1 + a^2}} \kappa^{(1)} E,
\]

(13)

and the variance is calculated by

\[
\frac{1}{\pi (1 + a)} \left( \kappa^{(1)} \right)^2 \int_{b = -a \pi}^{b = \pi} [\Delta \zeta (b) - E]^2 \, db,
\]

(14)

with \( E = \frac{1}{\pi (1 + a)} \int_{b = -a \pi}^{b = \pi} \Delta \zeta (b) \, db \). We emphasize again that deriving these results using a direct approach involves calculations over truncations of infinite spectra, thereby leading to estimates rather than rigorous results.

We are ready to introduce novel composites for which our analysis applies as well, and begin with laminates comprising non-linear soft layers [22, 30]. We consider waves propagating in such laminates when finitely deformed in a piecewise-homogeneous manner. By applying the theory of incremental elastic deformations [31], Eq. (1) is recovered as the dispersion relation of such “small on large” waves, and therefore the resultant spectrum is endowed with the torus representation. The physical and geometrical quantities entering Eq. (1) are now functions of the finite deformation, which thus renders the spectrum tunable. In addition to the validity of the previous results, our representation further provides a convenient tool for characterizing this tunability. This is demonstrated next, by way of example. The example considers transverse waves superposed on a plane deformation of an incompressible laminate. We denote the principle stretches in each phase by \( \lambda^{(p)} \) and \( 1/\lambda^{(p)} \), on account of incompressibility. The laminate direction considered is along the principal axis associated with \( \lambda^{(p)} \), such that \( h^{(p)} \) is related to the thickness before the deformation, \( H^{(p)} \), via \( h^{(p)} = \lambda^{(p)} H^{(p)} \). The velocity of transverse waves propagating in this direction is

\[
\epsilon^{(p)} = \sqrt{\frac{\hat{\mu}^{(p)}}{\rho^{(p)}}},
\]

(15)

where the instantaneous stiffness \( \hat{\mu}^{(p)} \), depends on the underlying deformation and the constitutive law of the phase. If a neo-Hookean law governs the layers behavior, we have that

\[
\hat{\mu}^{(p)} = \lambda^{(p)} \mu^{(p)},
\]

(16)

where \( \mu^{(p)} \) is the shear modulus in the limit of small strains. A simple calculation shows that \( \kappa^{(p)} \) and the flow direction are unaffected by the deformation, namely,

\[
\kappa^{(p)} = \frac{\epsilon^{(p)}}{h^{(p)}} = \sqrt{\frac{\lambda^{(p)} \mu^{(p)} / \rho^{(p)}}{\lambda^{(p)} H^{(p)} / \rho^{(p)}}} = \sqrt{\frac{\hat{\mu}^{(p)} / \rho^{(p)}}{H^{(p)}}}.
\]

(17)

To examine how the domain of \( \mathbb{D} \) is changed by the deformation, assume without loss of generality that \( \rho^{(1)} \mu^{(1)} > \rho^{(2)} \mu^{(2)} \); if \( \lambda^{(1)} > \lambda^{(2)} \) (resp. \( \lambda^{(1)} < \lambda^{(2)} \)), then \( \gamma \) is greater (resp. less) than its value before the deformation, and the area of \( \mathbb{D} \) increases (resp. decreases). Together with the observation made on \( a \) and \( \kappa^{(p)} \), it implies that frequencies are added to (resp. removed from) the boundaries of the gaps, without changing the mean frequency of each gap.
Consider next layers that are characterized by a Gentian model [32]. In this case, the instantaneous stiffness is

\[
\mu^{(p)} = \lambda^{(p)2} \mu^{(p)2} \left( 1 - \frac{\lambda^{(p)2} + \lambda^{(p)} - 2}{J_m^{(p)}} \right),
\]

(18)

where the material parameter \( J_m \in (0, \infty) \) models the rapid rise of stress in elastomers when approaching a limiting strain. Assume first that \( J_m^{(1)} = J_m^{(2)} \equiv J \) and \( \lambda^{(1)} = \lambda^{(2)} \equiv \lambda \). In such case, the flow direction and impedance contrast are not modified by the deformation; however, the flow rate, \( \frac{d \omega}{d \varphi} \), is multiplied by \( 1 - \left( \lambda^{2} + \lambda^{-2} - 2 \right) / J \). Consequently, the pertinent frequencies are multiplied by the inverse of this factor. Observing this factor is a monotonically decreasing function of \( \lambda \) with a range \( (0, 1) \) [33], implies that the frequency spectrum is shifted towards higher frequencies, and its gaps are rendered wider, by that factor. When \( J_m^{(1)} \neq J_m^{(2)} \) or \( \lambda^{(1)} \neq \lambda^{(2)} \), the flow direction changes with the deformation, and so does the impedance contrast. Thus, the spectrum is rendered tunable in a more intricate manner. The exploration of the specific way it takes effect depending on the relation between \( J_m^{(p)} \) and \( \lambda^{(p)} \) is beyond the scope of this example; however, we note that following the way the aforementioned relations enter Eq. (7), the flow lines will rotate either clockwise or counter-clockwise, and the length of their intersections with the resultant domain of \( \mathbb{D} \) will accordingly change.

The analysis of the resultant \( \Delta \omega \) is rendered simpler, in virtue of the torus universality, as for each \( \gamma \), the relation between \( \Delta \omega \) and \( a \) is unchanged. Therefore, one can calculate the resultant slope \( a \) in terms of \( J_m^{(p)} \) and \( \lambda^{(p)} \), and employ a fixed calculation of \( \Delta \omega / \sqrt{1 + a^2} \), to evaluate Eq. (9).

We continue with dielectric elastomers (DEs), a class of soft active materials. DEs undergo finite strains and change their physical properties by application of electric stimuli [34, 35]. The work in Ref. [36] has shown that under particular settings, the propagation of waves in finitely deformed DE laminates is also described by Eq. (1). Hence, the torus representation holds in this case as well, and subsequently, the validity of our previous observations is established. In particular, the torus representation provides a platform for an investigation of the effect the electric field has on the frequency spectrum.

We consider next magnetorehological elastomers (MREs) [37]. These materials consist of ferromagnetic particles embedded in a rubber-like matrix. Application of magnetic stimuli induces magnetic forces and moments on the inclusions. This changes the microstructure of the material, and, in turn, alters its configuration and stiffness. When the particles are disturbed in a chain-like manner, the material admits a laminated structure [38, 39]. We argue that our analysis also applies to MREs, in light of the similarly with DEs. First, we note that under a quasi magneto-electrostatic approximation, the governing electric and magnetic fields are differentially similar [40]. Second, the mechanical response of both MREs and DEs is governed by an elastomeric substance. The only difference is the relation between the magnetic load and the resultant stretch, on account of a different magnetic constitutive behavior. Therefore, under the same settings, the propagation of superposed waves is governed by the same dispersion relation derived for DEs. The applicability of our analysis thereby follows.

We complete this letter with a summary of our main conclusions, and a glance towards future challenges. We found that the frequency spectra of various 1D crystals admit a universal structure, independent of the geometry of their unit-cells and specific physical properties. This structure enabled us to derive universal properties of the spectra, and rigorously determine the gaps-density, their expected and maximal widths, and relate these to particular compositions. We showed that our conclusions successfully apply to certain multi-physical materials, of tunable spectra. We utilized our framework to characterize this tunability. Thus far, the results above were either unknown, or determined in an approximate manner.

Our future objectives are to extend this approach to analyze interesting generalizations of the considered systems. One such generalization is a crystal consisting of more than two constituents. In this case, the dispersion relation will depend on additional products [41] in the form of Eq. (4), as inferred from a transfer-matrix analysis [36, 41]. Our extended analysis will consequently require a torus whose dimensionality equals the number of constituents. \( \mathbb{N} \)-periodic media are also systems of major interest. In these composites, a closed-form expression for the dispersion relation is not available, and series-type solutions are sought [3, 7]. It is an imperative challenge to establish counterparts of the results reported herein for such materials.

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