On the Properties of Phononic Eigenvalue Problems

Amir Ashkan Mokhtari and Ankit Srivastava

Department of Mechanical, Materials, and Aerospace Engineering,
Illinois Institute of Technology, Chicago, IL, 60616 USA

(Dated: February 20, 2019)

In this paper we consider the phononic problem within the context of the spectral theorem. In doing so we present a unified understanding of the properties of the eigenvalues and eigenvectors which would emerge from any numerical method employed to compute such quantities. We show that the phononic problem can be cast into linear eigenvalue forms from which such quantities as frequencies ($\omega(\beta)$), wavenumbers ($\beta(\omega, n)$), and desired components of wavevectors ($\beta_3(\omega, \beta_\alpha)$) can be directly ascertained without resorting to searches or quadratic eigenvalue problems and that the relevant properties of such quantities can be determined apriori through the analysis of the associated operators. We further show how the Plane Wave Expansion (PWE) method may be extended to solve each of these eigenvalue forms, thus extending the applicability of the PWE method to cases beyond what have been considered till now. For the cases considered, we discuss relevant and important properties of the eigenvalue forms. This includes the space in which the eigenvalues are to be found, the relevant orthogonality conditions, the completeness (or non-completeness) of the basis and the need to form generalized eigenvectors for those phononic eigenvalue forms which are not normal. The techniques and results presented here are expected to apply to wave propagation in other periodic systems such as photonics.

Keywords: Spectral theorem, Phononics, Orthogonality, Scattering
I. INTRODUCTION

There has been considerable recent research interest in the field of wave propagation in periodic structures under the fields of photonics, phononics, and even metamaterials. Much of the progress in these fields depends upon the determination of wave propagation characteristics in such periodic systems. Historically, numerical efforts in this direction have been driven towards the calculation of the so-called bandstructure of the periodic system which is a graphical representation of the frequency-wavevector pairs which satisfy a certain kind of dispersion relationship for the system. Traditionally, such dispersion relations have been calculated through what we would call the conventional form of the eigenvalue problem – determining acceptable frequencies given a wavevector – termed \( \omega(k) \) systems. A host of numerical techniques have been devised to solve this particular form of the eigenvalue problem. This includes the Plane Wave Expansion (PWE) method, the multiple scattering method, variational techniques, FEM, and Finite Difference techniques.

Of late, there has been growing interest in the solution of the eigenvalue problem of periodic systems when the problem is not in a traditional form. The simplest of these cases is the solution of the \( \omega(\beta) \) eigenvalue form in the presence of dissipation. In this case, it turns out that the resulting frequencies for real assumed wavevectors are complex. A further complication which has been considered in literature is the determination of the wavenumber when frequency is given (termed \( \beta(\omega, n) \) form). The corresponding eigenvalue problem is most naturally quadratic in nature and, therefore, naturally more difficult to solve. In an algorithm for 1D systems was developed that provided dispersion curves for damped free wave motion based on frequencies and wavenumbers that are permitted to be simultaneously complex. The algorithm was applied to a viscously damped mass-in-mass metamaterial exhibiting local resonance. In their study, two eigenvalue problems were solved: Frequency solutions from linear eigenvalue problem, and wavenumber solutions from quadratic eigenvalue problem. As the latter problem is quadratic, a search algorithm was presented to find the wavenumber solutions for a given frequency. The problem can alternatively be converted into a linear eigenvalue form by using a state space representation. The resulting mixed-form of the elastodynamics problem has been considered in detail in the Finite Element literature (Least-Squares FEM) but its appearance in the phononics/photonic area is rare. Computational techniques used to solve such a problem in the area of phononics/photonic are, therefore, limited as well to what is called the Extended PWE method.

A further complication, rarely studied till now, which could be considered is the determination of one components of the wavevector when the other components and the frequency are given - termed \( \beta(\omega, n) \) problems. Such problems naturally emerge in cases where scattering in an interface are being studied. This is due to the fact that Snell’s law ensures that the components of the wavevector tangential to the interface are preserved and, therefore, there is a natural requirement to determine the remaining component when the preserved component is specified. Currently, there appears to exist no study in phononics which could directly solve this problem.

In this paper, we ask some basic questions pertaining to the phononic eigenvalue problems and propose some solutions. Foremost, is our attempt to analyze the phononic eigenvalue problems in the three different forms mentioned above through the lens of linear operators. This exercise reveals to us the basic properties of the eigenvalues and eigenvectors which can be expected from numerical calculations without actually doing any calculations. In all the eigenvalue forms, we are interested in determining the appropriate orthogonality conditions and whether the eigenvector basis is complete. In addition to the theoretical considerations, we also present extensions to the PWE method and give representative solutions for the eigenvalue forms considered.

This paper is organized as follows: in section II a brief introduction of the spectral theorem and properties of normal and self-adjoint operators are presented. We then investigate the properties of \( \omega(\beta) \) problem for different cases of material properties and also different types of wave number (real and complex) in section III. In section IV, the general problem of \( \beta(\omega) \) and the corresponding properties of its eigenvalues and eigenvectors are studied. One special case of this problem is the \( \beta_3(\omega, \beta_n) \) problem which is formulated in section IV.

II. EIGENVALUE PROPERTIES OF LINEAR OPERATORS

Here we are concerned with eigenvalue problems of the following form:

\[
Av = \lambda Bv
\]

where \( A, B \) are linear operators which act on an infinite-dimensional Hilbert space \( H \) of complex functions over which an inner product has been defined:

\[
\langle u, v \rangle = \int uv^\ast \, dx
\]
where \( u, v \in H \). The adjoint operator to \( A \), denoted by \( A^* \), is defined by:

\[
\langle Au, v \rangle = \langle u, A^* v \rangle
\]

The spectral theorem states some properties of the eigenvalues \( \lambda \) and the associated eigenvectors based upon the properties of the operators \( A, B \). Consider the case where \( A, B \) are normal operators:

\[
AA^* = A^* A; \quad |Av| = |A^* v|
\]

with similar relations for \( B \). If \( \lambda \) is an eigenvalue of \( A \) with associated eigenvector \( v \) \((Av = \lambda Bv)\) then

\[
|(A - \lambda B)v| = |(A - \lambda B)^* v| = 0,
\]

showing that \( \lambda^* \) is an eigenvalue of \( A^* \) with the same eigenvector \((A^*v = \lambda^* B^* v)\). If \( \lambda_1, \lambda_2 \) are two distinct eigenvalues with associated eigenvectors \( v, w \) then

\[
\lambda_1 \langle Bv, w \rangle = \langle Av, w \rangle = \langle v, A^* w \rangle = \langle v, \lambda_2^* B^* w \rangle = \lambda_2 \langle Bv, w \rangle
\]

showing that the eigenvectors are orthogonal \((\langle Bv, w \rangle = 0)\). Self-adjoint operators \((A = A^*)\) form a subset of normal operators and if \( A, B \) are self-adjoint and \( B \) is positive definite then the associated eigenvalues are real. In both cases the eigenvectors form a complete basis. A further result of importance to us can be proven by considering the finite dimensional matrix representations of the operators \( A, B \). Representing the matrix representations of \( A, B \) by \([A], [B]\), it is straightforward to show that if \( A \) is self-adjoint then \([A]\) is hermitian. Furthermore, if \( A \) is positive definite \((\langle Av, v \rangle > 0)\) then \([A]\) is also positive definite \((\langle x \rangle^1 [A] [x] > 0)\) where \(^\dagger\) represents conjugate transpose. Similar consideration holds for negative-definiteness as well. Now representing the generalized eigenvalue problem in matrix form:

\[
[A]\{v\} = \lambda [B]\{v\}
\]

Now if \([B]\) is positive definite then all its eigenvalues are positive. Since the eigenvalues of \([B]^{-1}\) are the inverse of the eigenvalues of \([B]\), its eigenvalues are also positive. Therefore, positive-definiteness of \([B]\) implies the positive-definiteness of \([B]^{-1}\). Now converting the generalized eigenvalue problem above into a standard eigenvalue problem:

\[
[C]\{v\} = \lambda\{v\}; \quad [C] = [B]^{-1}[A]
\]

Denoting \([B]^{-1} = [H]\) we have \((\{v\} [A])^\dagger [H][A]\{v\} = \{v\}^\dagger [A][H][A]\{v\} > 0\) since \([H]\) is positive definite and \([A]\) is hermitian. Now we have the generalized eigenvalue problem

\[
[H][A]\{v\} = \lambda\{v\}
\]

\[
{v}^\dagger [A][H][A]\{v\} = \lambda {v}^\dagger [A]\{v\}
\]

\[
\lambda = \frac{{v}^\dagger [A][H][A]\{v\}}{{v}^\dagger [A]\{v\}}
\]

showing that all eigenvalues \( \lambda \) of the generalized eigenvalue problem are negative since the numerator is positive and the denominator is negative. Therefore, in a eigenvalue problem \(Av = \lambda Bv\) where \( A \) is negative definite and self-adjoint and \( B \) is positive definite, all \( \lambda \) are real and negative.

### III. \( \omega(\beta) \) SOLUTIONS FOR A WAVE WITH A GIVEN WAVEVECTOR

Consider Bloch waves propagating in a phononic crystal in direction \( n \). The displacement and stress fields due to the wave will have the general form:

\[
u = \tilde{u} \exp[i(\omega t - \beta n \cdot x)]
\]

\[
\sigma = \tilde{\sigma} \exp[i(\omega t - \beta n \cdot x)]
\]

where \( \tilde{u}, \tilde{\sigma} \) are \( \Omega \)-periodic. \( \omega \) and \( \beta \) can both potentially assume real, imaginary, or complex values, however, only certain combinations are physically meaningful. First consider the usual form of the eigenvalue problem:

\[
(C_{ijkl} \tilde{u}_k,\ell - i\beta n_l C_{ijkl} \tilde{u}_k,\ell) - i\beta n_j C_{ijkl} \tilde{u}_k,\ell - \beta^2 n_i C_{ijkl} n_l \tilde{u}_k = \lambda \rho \tilde{u}_i
\]

where \( \lambda = -\omega^2 \), which is in the form

\[
A\tilde{v} = \lambda B\tilde{v}
\]
when one identifies \( \bar{v} \equiv \{ \bar{u} \} \). Now consider two \( \Omega \) periodic fields \( \bar{v}, \bar{w} \). The relevant inner product for the operator \( A \) is:

\[
\langle A\bar{v}, \bar{w} \rangle = \int \left[ (C_{ijkl}\bar{v}_{k,l} - i\beta n_l C_{ijkl}\bar{v}_{k,l} ) - i\beta n_j C_{ijkl}\bar{v}_{k,l} - \beta^2 n_j C_{ijkl}n_l \bar{v}_{k,l} \right] \bar{w}_i^* d\Omega
\]

Since \( C_{ijkl}, \bar{v}, \bar{w} \) are all \( \Omega \) periodic terms, the above can be transformed using Gauss theorem into:

\[
\langle A\bar{v}, \bar{w} \rangle = \int \bar{v}_k \left[ (C_{ijkl}\bar{w}_{i,j}^* + i\beta n_j C_{ijkl}\bar{w}_{i,j}^* ) + i\beta n_l C_{ijkl}\bar{w}_{i,l}^* - \beta^2 n_j C_{ijkl}n_l \bar{w}_i^* \right] d\Omega \equiv \langle \bar{v}, A^* \bar{w} \rangle
\]

showing that the adjoint operator \( A^* \) is:

\[
A^* \bar{w} = (C_{ijkl}^* \bar{w}_{i,j} - i\beta^* n_j C_{ijkl}^* \bar{w}_{i,j} ) + i\beta^* n_l C_{ijkl}^* \bar{w}_{i,l} - \beta^2 n_j C_{ijkl}^* n_l \bar{w}_i
\]

In what follows we will use \( C \) for the tensor \( C_{ijkl} \), \( n \) for the vector \( n_k \), and \( \bar{v} \) for the vector \( \bar{v}_k \). Tensor contraction to the right of \( C \) will represent contraction with respect to the last two indices and to the left will represent contraction with the the first two indices. Appropriate contractions are assumed without making them explicit. With this we have:

\[
|A\bar{v}|^2 = \langle A\bar{v}, A\bar{v} \rangle
\]

\[
|A^* \bar{w}|^2 = \langle A^* \bar{w}, A^* \bar{w} \rangle
\]

where \( \mathbf{a} = (\nabla \cdot C \nabla \bar{v} - \beta^2 n C \nabla \bar{v}) \) and \( \mathbf{b} = (\nabla \cdot C \nabla \bar{v} + n C \nabla \bar{v}) \). On the other hand we have:

\[
|A^* \bar{v}|^2 = \langle A^* \bar{v}, A^* \bar{v} \rangle
\]

\[
|A \bar{w}|^2 = \langle A \bar{w}, A \bar{w} \rangle
\]

where \( \mathbf{c} = (\nabla \cdot \nabla C^* - \beta^2 n \nabla C^* \bar{w}) \) and \( \mathbf{d} = (\nabla \cdot n \nabla C^* + \nabla \nabla C^* n) \). Therefore, in general, \( |A\bar{v}| \neq |A^* \bar{w}| \), or \( A \) is not a normal operator. However, for certain special cases \( A \) becomes a normal operator and the spectral theorem applies to it. The stiffness tensor \( C \) can always be separated into its hermitian and skew-hermitian parts \( C = H + N \) where \( H_{ijkl} = H_{ijkl} \) and \( N_{ijkl} = -N_{ijkl} \).

### A. Real \( \beta \)

a. \( C = H \): Consider the case when the skew-hermitian part is zero \( (N = 0) \). In this case, \( C_{ijkl}^* = C_{ijkl} \), and we have \( \mathbf{c} = (\nabla \cdot C \nabla C^* - \beta^2 n \nabla C^* \bar{w}) \) and \( \mathbf{d} = (\nabla \cdot n \nabla C^* + \nabla \nabla C^* n) \). If we further insist that \( \beta \) is real \( (\beta^* = \beta) \) then \( \mathbf{c} = \mathbf{a}, \mathbf{d} = \mathbf{b} \) and, in fact, \( |A\bar{v}| = |A^* \bar{w}| \) and \( A \) is a normal operator. Moreover, in this case the adjoint operator is

\[
A^* \bar{w} = (C_{ijkl} \bar{w}_{i,j} - i\beta n_j C_{ijkl} \bar{w}_{i,j} ) + i\beta n_l C_{ijkl} \bar{w}_{i,l} - \beta^2 n_j C_{ijkl} n_l \bar{w}_i
\]

showing that \( A^* = A \), or that \( A \) is a self-adjoint operator. Since the operator \( B \) is clearly self-adjoint (and, therefore, normal), the eigenvalue problem which emerges from assuming a real wavenumber in an elastodynamic system characterized by a stiffness tensor which respects the symmetry \( C_{ijkl}^* = C_{ijkl} \) is self adjoint. The eigenvalues, \( \lambda \), are, therefore, real and the corresponding frequencies \( \omega = \pm \sqrt{-\lambda} \) can be either real or imaginary (but not complex with
simultaneously nonzero real and imaginary parts). We further have:

\[ \langle A\bar{v}, \bar{v} \rangle = \int \left[ (C_{ijkl} \bar{v}_{k,l} - i\beta n_{ij} C_{ijkl} \bar{v}_{k,l} - \beta^2 n_{ij} C_{ijkl} n_{k,l} \bar{v}_{k,l} - \beta^2 n_{ij} C_{ijkl} n_{k,l} \bar{v}_{k,l}) \bar{v}^* d\Omega \right. \]

\[ = \int \left[ -\bar{v}^*_{i,j} C_{ijkl} \bar{v}_{k,l} - \beta^2 n_{ij} \bar{v}^*_i C_{ijkl} n_l \bar{v}_k + i\beta \bar{v}^*_{i,j} C_{ijkl} n_l \bar{v}_k - i\beta n_{ij} \bar{v}^*_i C_{ijkl} n_l \bar{v}_k \right] d\Omega \]

\[ = -\int \left[ \bar{v}^*_{i,j} - i\beta \bar{v}^*_{i,j} n_{ij} \right] C_{ijkl} \left[ \bar{v}_{k,l} + i\beta \bar{v}_k n_l \right] d\Omega \]

which is of the form \(-\int s_{ij} C_{ijkl} s_{kl}^* d\Omega\) when one identifies \(s_{ij} = \bar{v}^*_{i,j} - i\beta \bar{v}^*_{i,j} n_{ij}\). If we assume that the stiffness tensor is positive-definite (a normal assumption for conservative systems) then the integral is always less than zero showing that the operator \(A\) is negative definite as well \((\langle A\bar{v}, \bar{v} \rangle \leq 0)\). Since the operator \(B\) is clearly positive definite, this means that all the eigenvalues \(\lambda\) of the generalized eigenproblem under real \(\beta\) and a self-adjoint and positive definite \(C\) tensor will be negative. All the frequencies \(\omega = \sqrt{-\lambda}\) will, therefore, be purely real. As an academic point which is a corollary of this analysis, if \(C\) is negative definite then all frequencies will be imaginary since all \(\lambda\) will be positive and real.

\(\textbf{b. } \textbf{C} = \textbf{N}\): If the hermitian part of the stiffness tensor is zero \((H = 0)\) then \(C_{kl}^* = -C_{kl}\). In this case, \(c = (−\nabla \cdot C\nabla \bar{v} + \beta^2 \nabla C \nabla \bar{v})\) and \(d = (−\nabla \cdot C\nabla - nC \nabla \bar{v})\). If \(\beta\) is such that \(\beta^2 = \beta^2\) then we will have \(c = -a\) and \(d = -b\). Of course, in this situation we will have \(c \cdot c^* = a \cdot a^*\) and \(d \cdot d^* = b \cdot b^*\). Even in this case if \(\beta\) is real then it is clear that \(|A\bar{v}| = |A^*\bar{v}|\) and that \(A\) is a normal operator. In this case, we have:

\[ A^* \bar{w} = (-C_{klij} \bar{v}_{i,j} + i\beta n_{ij} C_{klij} \bar{w}_{i,j})_{,l} + i\beta n_{ij} C_{klij}^* \bar{w}_{i,j} + \beta^2 n_{ij} C_{klij} n_{k,l} \bar{w}_{i,l} \]

(18)

showing that \(A^* = A\). Therefore, unlike in the case where \(N = 0\), \(H = 0\) (for real \(\beta\)) leads to an eigenvalue problem which is not self-adjoint. It is, however, normal which means that the eigenvectors will be orthogonal and will form a complete basis. The eigenvalues, in this case, have no requirement of being real. Instead we have \(A^* = -A\) and, therefore,

\[ \lambda(Bv, v) = \langle Av, v \rangle = \langle v, A^* v \rangle = \langle v, -Av \rangle = -\lambda \langle v, Bv \rangle = -\lambda^* \langle Bv, v \rangle \]

(19)

showing that \(\lambda^* = -\lambda\). This, in turn, means that all eigenvalues of the problem will be strictly imaginary. Since \(\omega = \sqrt{-\lambda}\), the corresponding frequencies will be complex with equal nonzero real and imaginary parts.

\(\textbf{c. } \textbf{C} = \textbf{N} + \textbf{H}\): In this case, the tensors \(a, b\) can be divided into two parts: one resulting from \(H\) and the other resulting from \(N\). We can write \(a = a^b + a^\alpha\) and similarly for \(b\). Carrying out the same decomposition for \(c, d\), we can show that \(c = a^\alpha - a^\beta\) and \(d = b^\beta - b^\alpha\). As \(c \cdot c^* = a^\alpha a^\alpha^*\) and \(d \cdot d^* = b^\beta b^\beta^*\) then \(|A\bar{v}|^2 \neq |A^*\bar{v}|^2\) and the operator \(A\) is not normal and consequently not self-adjoint. In this case, the eigenvalues \(\lambda\) are complex which result in complex frequencies.

\section*{B. Imaginary and complex \(\beta\)}

Assuming \(\beta = i\beta_3\), we have \(c = (\nabla \cdot C\nabla \bar{v} + \beta_3^2 \nabla C \nabla \bar{v})\) and \(d = (\nabla \cdot C\nabla + nC \nabla \bar{v})\) and \(a = (\nabla \cdot C\nabla + \beta_3^2 \nabla C \nabla \bar{v})\) and \(b = (\nabla \cdot C\nabla + nC \nabla \bar{v})\). Then \(c = a, d = b\), however as \(\beta^* \neq i\beta\), then from Eqs. (13)-(16), we have \(|A\bar{v}|^2 \neq |A^*\bar{v}|^2\). When \(\beta = \beta_R + i\beta_3\), then \(c \neq a, d \neq b\) and consequently the operator is not normal when \(\beta\) is not real. In these cases, the eigenvalues are complex form and eigenvectors are not orthogonal with respect to the operator \(B\).

\section*{C. \(\omega(\beta)\) solutions using PWE}

Consider a periodic structure with the reciprocal-lattice vectors \(G = (G_1, G_2, G_3)\). The material properties and field variables can be expanded using Fourier series as follows:

\[ \alpha(r) = \sum_G \alpha^G e^{iG \cdot r} \]

(20)

\[ f(r) = e^{-i\omega t} \sum_G f^G e^{i(G+K) \cdot r} \]

(21)
where $\alpha$ can be any of $\{\rho, C, \mu, \lambda\}$ and $f$ can be $\{u, \sigma\}$. Also, $r = (x_1, x_2, x_3)$ is the position vector and $K = \beta(n_1, n_2, n_3)$ is the wave vector. Substituting the material properties and displacement field in the elastodynamics equation of motion we have:

$$
\nabla \left[ \sum_G C^G : \nabla \left( \sum_G u^G e^{i(G + \tilde{G} + K) \cdot r} \right) \right] = -\omega^2 \sum_G \rho^G \sum_G u^G e^{i(G + \tilde{G} + K) \cdot r} \tag{22}
$$

The bandstructure for an in-plane wave propagation in a square unit cell with a circular hole for different cases of $C = H, C = N$ and $C = N + H$ are shown in Fig. (1). In Fig. (1-b) $C = N$ and as we can see, the real and imaginary parts of the frequency are equal. In Figs. (1-c,d) the real and imaginary parts of the frequency are plotted when 10% loss is added to the Young modulus. We can see that the real part of the frequency is equal to the case of $C = H$ and the imaginary part of the frequency also has the same general shape but with a different amplitude.

**FIG. 1.** $\omega(\beta)$ plot for the 2D in-plane wave propagation for: (a) $C = H$ (b) $C = N$ (c) real and (d) imaginary parts of frequency for $C = N + H$

**IV. $\beta(\omega)$ SOLUTIONS FOR A WAVE AT A GIVEN FREQUENCY**

As a slight modification of the problem, we can seek $\beta$ solutions given frequency $\omega$ and a direction $n$. To derive the appropriate eigenvalue form we write the elastodynamic equations as:

$$
\sigma_{ij,j} = -\omega^2 \rho u_i
\quad \sigma_{ij} = C_{ijkl} u_{k,l} \tag{23}
$$
Now considering $\mathbf{u} = \hat{\mathbf{u}} \exp(-i\beta n, x_i)$ and $\mathbf{\sigma} = \hat{\mathbf{s}} \exp(-i\beta n, x_i)$:

\[
\begin{align*}
\bar{s}_{ij,j} - i\beta n_j s_{ij} &= -\omega^2 \rho \bar{u}_i \\
\bar{s}_{ij} &= C_{ijkl}(\bar{u}_{k,l} - i\beta \bar{u}_k n_l)
\end{align*}
\] (24)

which after some rearrangement can be written as:

\[
A\phi = \beta B\phi
\]

where $\phi \equiv \{\hat{\mathbf{u}} \ \hat{\mathbf{s}}\}^T$ and the linear operators are given by:

\[
A = \begin{bmatrix}
\omega^2 \rho(\cdot) & \nabla \cdot (\cdot) \\
-C : \nabla(\cdot) & I
\end{bmatrix}; \quad B = i \begin{bmatrix} 0 & (\cdot) \cdot n \\
-C : (\cdot) \otimes n & 0 \end{bmatrix}
\] (25)

If $\mathbf{u}$ is vector valued $\mathbf{u}$ then the inner product is defined by:

\[
\langle \mathbf{u}, \mathbf{v} \rangle = \int u_i v_i^* dx
\] (26)

and the adjoint operator to a linear operator $M$, denoted by $M^\dagger$, is defined by:

\[
\langle M(\mathbf{u}), \mathbf{v} \rangle = \langle \mathbf{u}, M^\dagger(\mathbf{v}) \rangle
\] (27)

Operator $A$ is self adjoint if $A = A^\dagger$. Identifying $\psi \equiv \{\hat{\mathbf{u}} \ \hat{\mathbf{s}}\}^T$ we have:

\[
\langle B(\phi), \psi \rangle = \int -iC_{ijkl}\bar{u}_k n_l \bar{s}_{ij}^* + in_j\bar{s}_{ij}\bar{u}_i^* dx = \langle \phi, B^\dagger(\psi) \rangle
\] (28)

so the adjoint of operator $B$ is:

\[
B^\dagger = \begin{bmatrix} 0 & i[(\cdot) : \mathbf{C}^*] \cdot n \\
-i(\cdot) \otimes n & 0 \end{bmatrix}
\] (29)

Since $B \neq B^\dagger$, operator $B$ is not self-adjoint. For operator $A$ we have:

\[
\langle A\phi, \psi \rangle = \int \left[ \bar{s}_{ij,j}\bar{u}_i^* + \omega^2 \rho \bar{u}_i \bar{s}_{ij}^* + \bar{s}_{ij}\bar{s}_{ij}^* - C_{ijkl}\bar{u}_{k,l}\bar{s}_{ij}^* \right] dx
\]

\[
= \int \left[ -\bar{s}_{ij}\bar{u}_{i,j}^* + \omega^2 \rho \bar{u}_i \bar{s}_{ij}^* + \bar{s}_{ij}\bar{s}_{ij}^* + C_{ijkl}\bar{u}_i \bar{s}_{ij,l}^* \right] dx
\]

\[
= \int \left[ ((C_{ijkl}\bar{s}_{kl})^* + \omega^2 \rho \bar{u}_i^*)\bar{u}_i - (\bar{u}_{i,j}^* - \bar{s}_{ij}^*)\bar{u}_{i,j} \right] dx = \langle \phi, A^\dagger(\psi) \rangle
\] (30)

Thus we have:

\[
A^\dagger = \begin{bmatrix} \omega^2 \rho(\cdot) & \nabla \cdot [\mathbf{C}^* : (\cdot)] \\
-\nabla \cdot (\cdot) & I \end{bmatrix}
\] (31)

In the above, it should be noted that the surface integral terms disappear since $\phi, \psi$ are $\Omega-$periodic. Since $A \neq A^\dagger$, operator $A$ is also not self-adjoint. It follows that the eigenvalues are complex and the associated eigenvectors are not orthogonal. To check whether the operator $A$ is normal or not, we have:

\[
|A\hat{\mathbf{v}}|^2 = \langle A\hat{\mathbf{v}}, A\hat{\mathbf{v}} \rangle = \int \left[ \omega^2 \rho \bar{u} + \nabla \cdot \bar{s}, -C : \nabla \bar{u} + \bar{s} \right] \cdot \left[ \omega^2 \rho \bar{u}^* + \nabla \cdot \bar{s}^*, -C^* : \nabla \bar{u}^* + \bar{s}^* \right] dx = \int \left[ (\omega^2 \rho)(\omega^2 \rho^*)\bar{u} \cdot \bar{u}^* + (\omega^2 \rho^*)\bar{u} \cdot \bar{s}^* + (\omega^2 \rho^*)\bar{s} \cdot \bar{u}^* + \bar{u} \cdot \bar{s} \cdot \nabla \cdot \bar{s}^* \right] dx + \int \left[ C : \nabla \bar{u} \cdot C^* : \nabla \bar{u}^* - C : \nabla \bar{u} \cdot \bar{s}^* - \bar{s} \cdot C^* : \nabla \bar{u}^* + \bar{s} \cdot \bar{s}^* \right] dx
\] (32)

\[
(33)
\]
two of the three components of the wavevector $\beta$.

By substituting the Fourier expansion of stress and displacement in to the above equation we have:

$$|A^\dagger \bar{v}|^2 = \langle A^\dagger \bar{v}, A^\dagger \bar{v} \rangle =$$

$$\int [\omega^2 \rho \bar{u} + \nabla \cdot [C^* : \bar{s}], \nabla \bar{u} + \bar{s} \cdot [\omega^2 \rho \bar{u}^* + \nabla \cdot [C^* : \bar{s}^*], \nabla \bar{u}^* + \bar{s}^*] dx$$

$$= \int [(\omega^2 \rho)(\omega^2 \rho^*) \bar{u} \cdot \bar{u}^* + (\omega^2 \rho^*) \bar{u} \cdot \nabla [C^* : \bar{s}] + (\omega^2 \rho) \nabla \cdot [C^* : \bar{s}^*] \cdot \bar{u}^* + \nabla \cdot [C^* : \bar{s}^*] \cdot \nabla \bar{u}^* + \bar{s} \cdot \bar{s}^*] dx$$

$$+ \int [\nabla \bar{u} \cdot \nabla \bar{u}^* + \nabla \bar{u} \cdot \bar{s}^* + \bar{s} \cdot \nabla \bar{u}^* + \bar{s}^*] dx$$  \hspace{1cm} (34)

As $|A\bar{u}|^2 \neq |A^\dagger \bar{v}|^2$ thus the operator $A$ is not normal and consequently its eigenvectors don’t form a complete basis.

### A. $\beta(\omega)$ solutions using PWE

This problem is generally a quadratic eigenvalue problem, but we can re-write it as mixed linear eigenvalue problem:

$$\nabla \cdot \sigma = \rho \bar{u}$$  \hspace{1cm} (35)

$$\sigma = C : \nabla \bar{u}$$  \hspace{1cm} (36)

By substituting the Fourier expansion of stress and displacement into the above equation we have:

$$\sum_i \hat{G}_i + \beta n_j \sigma_{ij} G^{G+K}_i \cdot r = -\omega^2 \sum_i \rho G^{G} \sum_j u_j \hat{G} \cdot e^{(G+G+K)_i \cdot r}$$

$$\sum_i \sigma_{ij} G^{G+K}_i \cdot r = \sum_i C_{ijkl} G^{G+K} \cdot u_k \hat{G} \cdot e^{(G+G+K)_i \cdot r}$$  \hspace{1cm} (37)

$$\sum_i \sigma_{ij} G^{G+K}_i \cdot r$$  \hspace{1cm} (38)

Multiplying both sides of the equations by $e^{-i(G+K)_i \cdot r}$ and integrating over the unit cell, and also by separating the terms which contain $\beta$, we have the following:

$$\sum_i \hat{G}_i \sigma_{ij} G^{G} = -i \beta n_j \sigma \hat{G}$$  \hspace{1cm} (39)

$$\sigma_{ij} G^{G} - i \sum_i C_{ijkl} G^{G} \cdot u_k \hat{G} \cdot e^{i(G+G+K)_i \cdot r} = \sum_i \beta C_{ijkl} n_i \hat{G} \cdot e^{-i(G+G+K)_i \cdot r}$$  \hspace{1cm} (40)

To use this formulation in an example, the complex bandsructure for an out-of-plane wave in a square unit cell of length 1 with a circular inclusion of radius 0.3 is plotted in Fig. (2). The complex bandstructer in Fig. (2a) is for a linear elastic material case, in which only two branches for the evanescent waves with pure imaginary wavemumber are plotted (among infinite number of evanescent waves). The first complex branch has the imaginary value of zero in the pass bands and a non zero value when in the band gap (where the real part is equal to $\pi$). The second complex branch corresponds to the largest eigenvalue with zero real part at each frequency. The bandstructure in Fig. (2b) is for the same unit cell but the viscoelastic matrix with the following complex modulus:

$$\mu(\omega) = \frac{\mu_\infty + \mu_0 \tau^2 \omega^2}{1 + \tau^2 \omega^2} - i \frac{(\mu_\infty - \mu_0) \tau \omega}{1 + \tau^2 \omega^2}$$  \hspace{1cm} (41)

where $\mu_\infty = \alpha \mu_0$ and $\mu_0 = 1.33e9$ $\alpha = 0.7$, $\tau = 0.0001$. As the stiffness tensor is frequency dependent in the viscoelastic materials, the $\omega(\beta)$ formulation cannot solve this problem directly, however, it is easy to solve it using the linear eigenvalue formualtion of $\beta(\omega)$. In some studies only the real part of the shear modulus is used to compare the bandgap behavior, however in Fig. (2b) both storage and loss modules are used. As one can see, for the viscoelastic case, pure real solutions cannot be predicted and the eigenvalues are complex. Also, the bandgap region is not apparent.

### B. $\beta_3(\omega, \beta_\omega)$ solutions

Now we consider another kind of the phononic eigenvalue problem. In this case we are given the frequency $\omega$ and two of the three components of the wavevector $\beta = \{\beta_1, \beta_2, \beta_3\}$. Without any loss of generality we assume that $\beta_1, \beta_2$
are known. The fields are of the form $u = \bar{u} \exp(-i\beta x_i)$ and $\sigma = \bar{s} \exp(-i\beta x_i)$. Denoting by greek letters the indices 1, 2 and by roman the indices 1, 2, 3 we can separate the equations of motion into the following:

$$\bar{s}_{ij,j} - i\beta_\alpha \bar{s}_{ij,\alpha} + \omega^2 \bar{\rho}_{ij} \bar{u}_i = i\beta_3 \bar{s}_{ij,3}$$

$$\bar{s}_{ij} - C_{ijkl}\bar{u}_{k,l} + iC_{ijkl}\beta_\alpha \bar{u}_k = -iC_{ijkl}\beta_3 \bar{u}_k$$

(42)

These equations can be cast in the generalized eigenvalue form by identifying two new vectors. Specifically we consider

$$\phi = \beta_3 B \phi$$

where $\phi \equiv \{\bar{u} \bar{s}\}^T$ and $A$, $B$ are defined as:

$$A = \begin{bmatrix} \omega^2 \rho(\gamma) & \nabla \cdot (\gamma) - i(\gamma) \cdot n \\ -C : \nabla (\gamma) + iC : (\gamma) \otimes n \end{bmatrix} \quad B = \begin{bmatrix} 0 & i(\gamma) \cdot n \\ -iC : (\gamma) \otimes n & 0 \end{bmatrix}$$

(43)

Now we have:

$$\langle B(\phi), \psi \rangle = \int \{\bar{u}_i \bar{s}_{ij}\} \left[ \frac{in\bar{s}_{ij}}{-iC_{ijkl}\bar{u}_{k,l}} \right] dx = \int \left[ -i\bar{s}_{ij}^* C_{ijkl} \bar{u}_{k,l} n_i + i\bar{u}_i n_j \bar{s}_{ij} \right] dx = \langle \phi, B^\dagger(\psi) \rangle$$

(44)

The adjoint of operator $B$ is then:

$$B^\dagger = \begin{bmatrix} 0 & i(\gamma) : C^* \cdot n \\ -i(\gamma) \otimes n & 0 \end{bmatrix}$$

(45)

Since $B \neq B^*$, operator $B$ is not self-adjoint. For operator $A$ we have:

$$\langle A(\phi), \psi \rangle = \int \left[ \bar{u}_i^* \bar{s}_{ij,j} - i\bar{u}_i^* \gamma_j \bar{s}_{ij,\alpha} + \omega^2 \bar{\rho}_{ij} \bar{u}_i + \bar{s}_{ij}^* \bar{s}_{ij,\gamma} - \bar{s}_{ij}^* C_{ijkl} \bar{u}_{k,l} + i\bar{s}_{ij}^* C_{ijkl} \gamma \bar{u}_k \right] dx$$

$$= \int \left[ -\bar{u}_i^* \gamma_j \bar{s}_{ij,\alpha} + \omega^2 \bar{\rho}_{ij} \bar{u}_i + \bar{s}_{ij} \bar{s}_{ij,\gamma} + (\bar{s}_{ij}^* C_{ijkl}) \bar{u}_{k,l} + i\bar{s}_{ij}^* C_{ijkl} \gamma \bar{u}_k \right] dx$$

$$= \int \left[ (\omega^2 \bar{\rho}_{ij} + (\bar{s}_{kl}^* C_{klij}) \gamma) \bar{u}_i + (\bar{s}_{ij}^* \gamma_j + \bar{s}_{ij}^*) \bar{s}_{ij} \right] dx = \langle \phi, A^\dagger(\psi) \rangle$$

(46)

(47)

Its adjoint satisfies:

$$A^\dagger = \begin{bmatrix} \omega^2 \rho(\gamma) \nabla \cdot (\gamma) - i(\gamma) : C^* \cdot n \\ -\nabla(\gamma) + i(\gamma) \otimes n \end{bmatrix}$$

(48)

Since $A \neq A^*$, operator $A$ is also not self-adjoint. It follows that the eigenvalues $\beta_3$ are complex. Among these complex eigenvalues, there are a limited real eigenvalues which refer to the propagating waves in the structure. Also infinite
number of eigenvalues are pure imaginary which are evanescent waves. One should note that with formulation in Eq. 12, the matrix $B$ associated with the discretized version of the operator $B$ (using PWE, FEM, etc.) is generally singular and thus there are eigenvalues with the value of infinity. There are numerical methods in computational algebra\cite{30} which can remove these eigenvalues if one is interested. However, the eigenvalues with finite value can still be obtained as shown in Fig. 3.

C. PWE solution

By substituting Eqs. (20,21) into Eq. (12) we have the following:

$$i \sum_G (\hat{G}_j + \beta_j) \sigma_{ij} e^{i(\hat{G}+K) \cdot r} = -\omega^2 \sum_G \rho^G \sum_G u_i^G e^{i(\hat{G}+\hat{G}+K) \cdot r}$$

$$\sum_G \sigma_{ij} G^G e^{i(\hat{G}+K) \cdot r} = i \sum_G \frac{C_{ijkl}}{G} \sum_G (\hat{G}_l + \beta_l) u_k^G e^{i(\hat{G}+\hat{G}+K) \cdot r}$$

Assuming that $\beta_1$ and $\beta_2$ are given, we can re-write the above equation in the following way to form a generalized eigenvalue with $\beta_3$ as the eigenvalues and $\{u, \sigma\}$ as the eigenvectors:

$$i \sum_G [(\hat{G}_\alpha + \beta_\alpha) \sigma^{G\alpha} + \hat{G}_{3\sigma} \sigma^{G\alpha}] e^{i(\hat{G}+K) \cdot r} + \omega^2 \sum_G \rho^G \sum_G u_i^G e^{i(\hat{G}+\hat{G}+K) \cdot r} = -i \sum_G \beta_3 \sigma^{G\alpha} e^{i(\hat{G}+K) \cdot r}$$

$$\sum_G \sigma^{G\alpha} e^{i(\hat{G}+K) \cdot r} - i \sum_G \frac{C_{ijkl}}{G} (\hat{G}_\alpha + \beta_\alpha) u_k^G e^{i(\hat{G}+\hat{G}+K) \cdot r} - i \sum_G \frac{C_{ijkl}}{G} \sum_G (\hat{G}_{3\beta} + \beta_{3\beta}) u_k^G e^{i(\hat{G}+\hat{G}+K) \cdot r} =$$

$$i \sum_G \frac{C_{ijkl}}{G} \sum_G \beta_3 u_k^G e^{i(\hat{G}+\hat{G}+K) \cdot r}$$

Multiplying both sides of the equations by $e^{-i(\hat{G}+K) \cdot r}$ and integrating over the unit cell, Eqs. (51,52) are written as follows:

$$i [ (\hat{G}_\alpha + \beta_\alpha) \sigma^{G\alpha} + \hat{G}_{3\beta} \sigma^{G\alpha} ] + \omega^2 \sum_G \rho^G u_i^G e^{i(\hat{G}+K) \cdot r} = -i \beta_3 \sigma^{G\alpha}$$

$$\sigma^{G\alpha} - i \sum_G \frac{C_{ijkl}}{G} (\hat{G}_\alpha - \beta_\alpha) u_k^G e^{i(\hat{G}+K) \cdot r} - i \sum_G \frac{C_{ijkl}}{G} (\hat{G}_{3\beta} - \beta_{3\beta}) u_k^G e^{i(\hat{G}+K) \cdot r} = i \beta_3 \sum_G \frac{C_{ijkl}}{G} u_k^G e^{i(\hat{G}+K) \cdot r}$$

![FIG. 3. (a) $\beta_1 - \beta_2$ plot for propagating waves at $\omega = 3000$ (rad/s) (b) $\beta_1 - \beta_2$ plot for the evanescent waves with pure imaginary $\beta_2$ values](image)

In Fig. 3 the $\beta_2(\beta_1, \omega)$ problem for a layered composite and an in-plane wave propagation is solved. In Fig (a) two branches corresponding to the two propagating waves in the composite at $\omega = 3000$ (rad/s) are shown, and also four branches of the evanescent waves (pure imaginary $\beta_2$ values) are shown in Fig. (b). The application of this
problem is when a metamaterial is interfaced with a homogeneous medium. In this problem, the $\beta_1$ component of the wavenumber is known when a plane wave is incident at the interface from the homogeneous part. Thus the $\beta_2$ values should be calculated in order to find the propagating waves in the metamaterial part.

V. CONCLUSION

Different categories of phononic eigenvalue problems were studied in this paper. For each problem, the properties of its eigenvalues and eigenvectors were revealed by the means of spectral theorem. It was shown that for the $\omega(\beta)$ problem, when $\beta$ is real and also the stiffness tensor has a Hermitian form, the eigenvalues are real and negative and the corresponding eigenvectors are orthogonal. Also, when the stiffness tensor is skew-Hermitian, the eigenvalues are real but positive which leads to pure imaginary frequency values. In these cases, the eigenvectors form a complete basis for the displacement field. For other cases of complex wavenumber or non-Hermitian stiffness tensor, the operator is not normal (and, therefore, not self-adjoint.) The $\beta(\omega, n)$ problem was studied using a mixed formulation in which the eigenvectors are made of both displacement and stress components and which results in the conversion of the quadratic eigenvalue problem to a linear one. It was shown that using the mixed formulation, the resulted operators are not normal. Consequently, even in the absence of damping, the eigenvalues are complex. The wavenumbers, therefore, correspond to both propagating and evanescent modes. Another important case considered is the $\beta_3(\omega, \beta_\alpha)$ problem which is especially useful for analyzing scattering problems. A mixed formulation was presented for this case which enables the direct determination of all the components of the wavenumber which would be required in a Snell’s law setting.

ACKNOWLEDGMENTS

A.S. acknowledges support from the NSF CAREER grant #1554033 to the Illinois Institute of Technology and NSF grant #1825354 to the Illinois Institute of Technology

* Corresponding Author
† asriva13@iit.edu

1 Sia Nemat-Nasser, “Anti-plane shear waves in periodic elastic composites: band structure and anomalous wave refraction,” in [Proc. R. Soc. A] Vol. 471 (The Royal Society, 2015).
2 Gal Shmuel and Ram Band, “Universality of the frequency spectrum of laminates,” Journal of the Mechanics and Physics of Solids 92, 127–136 (2016).
3 Qianli Chen and Ahmed Elbanna, “Modulating elastic band gap structure in layered soft composites using sacrificial interfaces,” Journal of Applied Mechanics 83, 111009 (2016).
4 Pierre A. Deymier, ed., [Acoustic Metamaterials and Phononic Crystals] (Springer Berlin Heidelberg, 2013).
5 K. M. Ho, C. T. Chan, and C. M. Soukoulis, “Existence of a photonic gap in periodic dielectric structures,” Physical Review Letters 65, 3152–3155 (1990).
6 Jun Mei, Zhengyou Liu, and Chunyin Qiu, “Multiple-scattering theory for out-of-plane propagation of elastic waves in two-dimensional phononic crystals,” Journal of Physics: Condensed Matter 17, 3735–3757 (2005).
7 M. Kafesaki and E. N. Economou, “Multiple-scattering theory for three-dimensional periodic acoustic composites,” Physical Review B 60, 11993–12001 (1999).
8 Ankit Srivastava and Sia Nemat-Nasser, “Mixed-variational formulation for phononic band-structure calculation of arbitrary unit cells,” Mechanics of Materials 74, 67–75 (2014).
9 Yan Lu and Ankit Srivastava, “Variational methods for phononic calculations,” Wave Motion 60, 46–61 (2016).
10 Yan Lu and Ankit Srivastava, “Combining plane wave expansion and variational techniques for fast phononic computations,” Journal of Engineering Mechanics 143, 04017141 (2017).
11 Steven R White, John W Wilkins, and Michael P Teter, “Finite-element method for electronic structure,” Physical Review B 39, 5819 (1989).
12 Istvan A Veres and Thomas Berer, “Complexity of band structures: Semi-analytical finite element analysis of one-dimensional surface phononic crystals,” Physical Review B 86, 104304 (2012).
13 Anne-Christine Hladky-Hennion and Jean-Nol Decarpigny, “Analysis of the scattering of a plane acoustic wave by a doubly periodic structure using the finite element method: Application to Alberich anechoic coatings,” The Journal of the Acoustical Society of America 90, 3356–3367 (1991).
14 M.I. Hussein, “Reduced bloch mode expansion for periodic media band structure calculations,” Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science 465, 2825 (2009).
Yukihiro Tanaka, Yoshinobu Tomoyasu, and Shin ichiro Tamura, “Band structure of acoustic waves in phononic lattices: Two-dimensional composites with large acoustic mismatch,” Physical Review B 62, 7387–7392 (2000).

CT Chan, QL Yu, and KM Ho, “Order-n spectral method for electromagnetic waves,” Physical Review B 51, 16635 (1995).

Mahmoud I. Hussein, “Theory of damped bloch waves in elastic media,” Physical Review B 80 (2009), 10.1103/physrevb.80.212301.

Mahmoud I. Hussein and Michael J. Frazier, “Band structure of phononic crystals with general damping,” Journal of Applied Physics 108, 093506 (2010).

Michael J. Frazier and Mahmoud I. Hussein, “Viscous-to-viscoelastic transition in phononic crystal and metamaterial band structures,” The Journal of the Acoustical Society of America 138, 3169–3180 (2015).

Michael J. Frazier and Mahmoud I. Hussein, “Generalized bloch’s theorem for viscous metamaterials: Dispersion and effective properties based on frequencies and wavenumbers that are simultaneously complex,” Comptes Rendus Physique 17, 565–577 (2016).

Vincent Laude, Younes Achaoui, Sarah Benchabane, and Abdelkrim Khelif, “Evanescent bloch waves and the complex band structure of phononic crystals,” Physical Review B 80 (2009), 10.1103/physrevb.80.092301.

Rayisa P. Moiseyenko and Vincent Laude, “Material loss influence on the complex band structure and group velocity in phononic crystals,” Physical Review B 83 (2011), 10.1103/physrevb.83.064301.

Erik Andreassen and Jakob S. Jensen, “Analysis of phononic bandgap structures with dissipation,” Journal of Vibration and Acoustics 135, 041015 (2013).

A.O. Krushynska, V.G. Kouznetsova, and M.G.D. Geers, “Visco-elastic effects on wave dispersion in three-phase acoustic metamaterials,” Journal of the Mechanics and Physics of Solids 96, 29–47 (2016).

Max D. Gunzburger and Pavel B. Bochev, Least-Squares Finite Element Methods (Springer New York, 2009).

Young-Chung Hsue, Arthur J. Freeman, and Ben-Yuan Gu, “Extended plane-wave expansion method in three-dimensional anisotropic phononic crystals,” Physical Review B 72 (2005), 10.1103/physrevb.72.195118.

Ankit Srivastava and John R Willis, “Evanescent wave boundary layers in metamaterials and sidestepping them through a variational approach,” in Proc. R. Soc. A, Vol. 473 (The Royal Society, 2017) p. 20160765.

Xingyi Zhu, Sheng Zhong, and Hongduo Zhao, “Band gap structures for viscoelastic phononic crystals based on numerical and experimental investigation,” Applied Acoustics 106, 93–104 (2016).

Y.P. Zhao and P.J. Wei, “The band gap of 1d viscoelastic phononic crystal,” Computational Materials Science 46, 603–606 (2009).

David S. Watkins, The Matrix Eigenvalue Problem (Society for Industrial and Applied Mathematics, 2007).