Effective speed of sound in phononic crystals

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A new formula for the effective quasistatic speed of sound \( c \) in 2D and 3D periodic materials is reported. The approach uses a monodromy-matrix operator to enable direct integration in one of the coordinates and exponentially fast convergence in others. As a result, the solution for \( c \) has a more closed form than previous formulas. It significantly improves the efficiency and accuracy of evaluating \( c \) for high-contrast composites as demonstrated by a 2D example with extreme behavior.

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I. INTRODUCTION

Long-standing interest in modeling effective elastic properties of composites with microstructure has substantially intensified with the emerging possibility of designing periodic structures in air\textsuperscript{1,2} and in solid\textsuperscript{3} to form phononic crystals and other exotic metamaterials, which open up exciting application prospects ranging from negative index lenses to small scale multiband phononic devices\textsuperscript{1,2}. This new prospective brings about the need for fast and accurate computational schemes to test ideas in silico. The most common numerical tool is the Fourier or plane-wave expansion method (PWE). It is widely used for calculating various spectral parameters including the effective quasistatic speed of sound in acoustic\textsuperscript{2} and elastic\textsuperscript{3} phononic crystals. At the same time, the PWE calculation is known to face problems when applied to high-contrast composites\textsuperscript{1,2}, which are of especial interest for applications. Particularly riveting is the case where a soft ingredient is embedded in a way breaking the connectivity of densely packed regions of stiff ingredient. Physically speaking, the speed of sound, which is large in a homogeneously stiff medium, should fall dramatically when even a small amount of soft component forms a ‘quasi-insulating network’. Note that this case, which implies a strong effect of multiple interactions, is also ungainly for the multiple-scattering approach\textsuperscript{1,2}. The purpose of present Letter is to highlight a new method for evaluating the quasistatic effective sound speed \( c \) in 2D and 3D phononic crystals. The idea is to recast the wave equation as a 1st-order ‘ordinary’ differential system (ODS) with respect to one coordinate (say \( x_1 \)) and to use a monodromy-matrix operator defined as a multiplicative (or path) integral in \( x_1 \). By this means, we derive a formula for \( c \) whose essential advantages are an explicit integration in \( x_1 \) and an exponentially small error of truncation in other coordinate(s). Both these features of the analytical result are shown to significantly improve the efficiency and accuracy of its numerical implementation in comparison with the conventional PWE calculation, which is demonstrated for a 2D steel/epoxy square lattice. The power of the new approach is especially apparent at high concentration \( f \) of steel inclusions, where the effective speed \( c \) displays a steep, near vertical, dependence for \( f \approx 1 \), a feature not captured by conventional techniques like PWE.

II. EFFECTIVE SPEED: 2D ACOUSTIC WAVES

A. SETUP. Consider the scalar wave equation

\[
\nabla \cdot (\mu \nabla v) = -\rho \omega^2 v, \tag{1}
\]

for time-harmonic shear displacement \( v(x,t) = v(x)e^{-i\omega t} \) in a 2D solid continuum\textsuperscript{2} with \( T \)-periodic density \( \rho(x) \) and shear coefficient \( \mu(x) \). Assume a square unit cell \( T = \sum t_i a_i = [0,1)^2 \) with unit translation vectors \( a_1, a_2 \) taken as the basis for \( x = \sum x_i a_i \). Imposing the Floquet condition \( v(x) = u(x)e^{ik \cdot x} \) where \( u(x) \) is periodic and \( k = k \cdot \kappa (|k| = 1) \), Eq. (1) becomes

\[
(C_0 + C_1 + C_2)u = \rho \omega^2 u \quad \text{with} \quad C_0 u = -\nabla(\mu \nabla u), \quad C_1 u = -ik \cdot (\mu \nabla u + \nabla(\mu u)), \quad C_2 u = k^2 \mu u. \tag{2}
\]

Regular perturbation theory applied to (2) yields the effective speed \( c(\kappa) \approx \lim_{\omega,k \to 0} \omega(\kappa)/k \) in the form\textsuperscript{3}

\[
c^2(\kappa) = \mu_{\text{eff}}(\kappa)/\langle \rho \rangle, \quad \mu_{\text{eff}}(\kappa) = \langle \mu \rangle - M(\kappa) \tag{3}
\]

\[M(\kappa) = \sum_{i,j=1}^2 M_{ij} \kappa_i \kappa_j, \quad M_{ij} = (C_0^{-1} \partial_i \mu, \partial_j \mu) = M_{ji},\]

where \( \partial_i \equiv \partial/\partial x_i \), spatial averages are defined by

\[
\langle f \rangle \equiv \frac{1}{T} \int_T f(x) dx \quad ( = \langle f \rangle_{L^2}, \quad \langle f \rangle_i \equiv \int_0^1 f(x) dx_i), \tag{4}
\]

and \( \langle \cdot, \cdot \rangle \) denotes the scalar product in \( L^2(T) \) so that \( \langle f, h \rangle = \langle fh^* \rangle \) (* means complex conjugation). The difficulty with (3) is that it involves the inverse of a partial differential operator \( C_0 \). One solution is to apply a double Fourier expansion to \( C_{0-1} \) and \( \partial_x \mu \) in (3). This leads to the PWE formula for the effective speed\textsuperscript{2} which is expressed via infinite vectors and the inverse of the infinite matrix of Fourier coefficients of \( \mu(x) \). Numerical implementation of the PWE formula requires dealing with large dense matrices, especially in the case of high-contrast composites for which the PWE convergence is slow (see §IV). An alternative "brute force" procedure of
the scaling approach is to numerically solve the partial 
differential equation $C_0 h = \partial_t \mu$ for the 1-periodic func-
tion $h(x)$ (e.g. via the boundary integral method). 

The new approach proposed here leads to a more effi-
cient formula for $c$ based on direct analytical integration 
in one coordinate direction. There are two ways of doing 
so. The first proceeds from the ODS form of the wave 
equation (1), itself, which means ‘skipping’ (3). This is 
convenient for deriving $c(\kappa)$ in the principal direc-
tions $\kappa \parallel a_{1,2}$, see §IIB. The second method is more 
closely related to the conventional PWE and scaling ap-
proaches related to the conventional PWE and scaling ap-
proaches (5) and hence (6) [1]. This is basi-
cally equivalent to the former method, but enables an 
easier derivation of the off-diagonal component $M_{12}$ for 
the anisotropic case, see §IIC.

B. Wave speed in the principal directions. The wave 
equation (1) may be recast as

$$\eta' = Q \eta \quad \text{with} \quad A = - \partial_2 (\mu \partial_2),$$

$$Q = \left( \begin{array}{cc} \omega & -\mu \omega^2 \mu^{-1} \\ 0 & -1 \end{array} \right), \quad \eta(x) = \left( \begin{array}{c} v \\ \mu' \end{array} \right).$$

where $\partial_t$ stands for $\partial_t$. The solution to Eq. (5) for initial 
data $\eta(0, x) \equiv \eta(0, \cdot)$ at $x_1 = 0$ is

$$\eta(x_1, \cdot) = M(x_1, 0) \eta(0, \cdot)$$

where $M$ is the matricant over a period, $\omega$ and $\kappa$ are 
the anisotropic case, see (3). This implies the eigenproblem

$$M(1, 0) w(k_1) = e^{ik_1} w(k_1).$$

where $M(1, 0)$ depends on $\omega$. Eq. (7) defines $k_1 = k_1(\omega)$ and hence $\omega = \omega(k_1)$, where $\omega^2$ is the eigenvalue of (1) 
with $v(x) = u(x) e^{ik_1 x_1}$. The effective speed $c(\kappa_1) = \lim_{\omega \to \omega(k_1)} \omega(k_1)$ can therefore be determined by applying perturbation theory to (7) as $\kappa_1 \to 0$. The asymptotic form of $M(1, 0)$ follows from definitions (5) and (6) as

$$M(1, 0) = M_0 + \omega^2 M_1 + O(\omega^4)$$

where

$$M_0 \equiv M_{0}[0, 1], \quad M_0(a, b) = \int_0^a (\mathcal{I} + Q_0 dx_1)$$

and

$$Q_0 = Q_{\omega = 0} = \left( \begin{array}{c} 0 \\ \mu^{-1} \end{array} \right).$$

$$M_1 = \int_0^1 M_0(x, 0) \left( \begin{array}{c} 0 \\ -\rho \end{array} \right) M_0(x, 0) dx_1.$$

Note the identities $Q_0 w_0 = 0$, $Q_0^T \tilde{w}_0 = 0$ and hence

$$M_0[a, b] w_0 = w_0, \quad M_0^+[a, b] \tilde{w}_0 = \tilde{w}_0 \quad (\forall a, b)$$

for $w_0 = (1 0)^T$, $\tilde{w}_0 = (0 1)^T$.

By (9), $w_0$ is an eigenvector of $M_0$ with the eigenvalue 1, and it can be shown to be a single eigenvector. Therefore

$$w(k_1) = w_0 + \kappa_1 w_1 + \kappa_1^2 w_2 + O(k_1^3)$$

and $\omega = \kappa_1 + O(k_1^2)$. Insert these expansions along with (8) in (7) and collect the first-order terms in $k_1$ to obtain

$$M_0 w_1 = w_1 + i w_0 \Rightarrow w_1 = i (M_0 - \mathcal{I})^{-1} w_0.$$  (10)

According to (9), $M_0 - \mathcal{I}$ has no inverse but is a one-to-
one mapping from the subspace orthogonal to $w_0$ onto 
the subspace orthogonal $w_0$, hence, $w_1$ exists and $w_0 \cdot w_1$ is uniquely defined. The terms of second-order in $k_1$ in (7) then imply

$$M_0 w_2 + c^2 M_1 w_0 = i w_1 + w_2.$$  (11)

Scalar multiplication on both sides by $\tilde{w}_0$ leads, with ac-
count for (9) and (8), to $c^2(\rho) = - i \langle \tilde{w}_0 \cdot w_1 \rangle_2$, whence by (10)

$$c^2(\kappa_1) = \langle \rho \rangle^{-1} \langle \tilde{w}_0 \cdot (M_0 - \mathcal{I})^{-1} w_0 \rangle_2.$$  (12)

where the notation $\langle \cdot \rangle_2$ is explained in (4). Interchanging variables $x_1 \rightleftharpoons x_2$ in the above derivation yields a similar result for $c(\kappa_2)$ as follows

$$c^2(\kappa_2) = \langle \rho \rangle^{-1} \langle \tilde{w}_0 \cdot (M_0 - \mathcal{I})^{-1} w_0 \rangle_1$$

$$\tilde{M}_0 = \int_0^1 (\mathcal{I} + \tilde{Q}_0 dx_2),$$

$$\tilde{Q}_0 = \left( \begin{array}{c} 0 \\ \mu^{-1} \end{array} \right), \quad \tilde{\mathcal{A}} = - \partial_1 \mu \partial_1.$$ 

The result for a rectangular lattice with $T = [0, T_1] \times 
[0, T_2]$ is obtained by replacing $x_1$ with $x_1 x_1 T_1$. 

C. The full matrix $M_{1j}$. The anisotropy of the effective speed $c(\kappa)$, i.e. its dependence on the wave normal $\kappa \equiv k/k_1$; is determined by the quadratic form

$$M(\kappa) = \sum_{i,j=1}^2 M_{ij} \kappa_i \kappa_j$$

(see Eq. (3)), and represented by the ellipse of (squared) slowness $c^{-2}(\kappa)$. Eqs. (12) and (13), which define $c(\kappa_i)$ and so $M_{ii}$, suffice for the case where $T$ is rectangular and $\mu(x)$ is even in (at least) one of $x_i$ so that the effective-slowness ellipse is

$$c^{-2}(\kappa) = \sum_{i=1}^2 c^{-2}(\kappa_i)$$

with the principal axes parallel to $a_1 \perp a_2$. Otherwise $c(\kappa)$ for arbitrary $\kappa$ requires finding the off-diagonal component $M_{12}$. For this purpose, with reference to (3), consider the equation

$$C_0 h = \partial_1 \mu$$  (14)

for 1-periodic $h(x)$. With the above notations this can be written as $(\mu h')' + Ah = \mu'$ or, more conveniently, $(\mu h')' = \mathcal{A} h$ with $\mathcal{A} = \mathcal{A} h$ with $h = h + x_1$. The latter is equivalent to

$$\xi' = \tilde{Q}_0 \xi \quad \text{where} \quad \xi = \left( \begin{array}{c} h \end{array} \right)$$  (15)
and \( Q_0 \) is given in (8). The general solution to (15) is
\[
\xi(x_1, \cdot) = M_0 [x_1, 0] \xi(0, \cdot),
\]
where \( M_0 [x_1, 0] \) is defined in (8), and \( \xi(0, \cdot) \) is the initial data at \( x_1 = 0 \). The periodicity of \( h \) implies \( \xi(1, \cdot) = \xi(0, \cdot) + w_0 \), while \( \xi(1, \cdot) = M_0 \xi(0, \cdot) \) by (16). Hence \( \xi(0, \cdot) = (M_0 - \mathcal{I})^{-1}w_0 \) and so (14) is solved by
\[
\xi(x_1, \cdot) = M_0 [x_1, 0] (M_0 - \mathcal{I})^{-1}w_0.
\]
Substituting (17) into the definition of \( M_{12} \) in (3) yields
\[
M_{12} = (c_0^{-1} \partial_1 \mu, \partial_1 \mu) = \langle \partial_2 \mu w_0 \cdot \xi \rangle = \langle \partial_2 \mu w_0 \cdot \xi \rangle + \langle M_0 [x_1, 0] (M_0 - \mathcal{I})^{-1}w_0 \rangle.
\]
Note that the formula (18) for \( M_{12} \) requires more computation than the formulas (12) and (13) for \( M_{ij} \). Interestingly, if the unit cell \( T \) is square, then, for an arbitrary (periodic) \( \mu(x) \), Eq. (18) can be circumvented by using the identity \( M_{12} = (M_{11} - M_{22})/2 \), where \( M_{ii} \) follow from Eqs. (12) and (13) applied to the square lattice obtained from the given one by turning it 45°.

**D. Discussion.** The two lines of attack outlined mentioned in §II.A are equivalent in that the formula (12) for the effective speed \( c(\kappa_1) \) in the principal direction can also be inferred from Eq. (9). Inserting the solution (17) of (14) defines the component \( M_{11} \) as
\[
M_{11} = \left( C^{-1} \partial_1 \mu, \partial_1 \mu \right) = \langle \mu' w_0 \cdot \xi \rangle - \langle x_1 \mu' \rangle.
\]
Integrating by parts each term in the last identity and using the periodicity of \( \mu(x) \) along with Eqs. (8) and (9), (15), (17) (see also the notation (4)) yields
\[
\langle \mu' w_0 \cdot \xi \rangle = \langle \mu' w_0 \cdot (M_0 - \mathcal{I})^{-1}w_0 \rangle = \langle \mu(0, x_2) \rangle_2 - \langle x_1 \mu' \rangle = \langle \mu \rangle - \langle \mu(x_1, x_2) \rangle_2 = \langle \mu \rangle - \langle \mu(0, x_2) \rangle_2.
\]
Thus, \( M_{11} = \langle \mu \rangle - \langle \mu \rangle \), which leads to (12). QED. Note that Eq. (18) is also obtainable via the monodromy matrix of the wave equation (1) (the approach of §II.B) with \( v(x) = u(x)e^{i k \cdot x} \) and \( k \parallel a_i \), but this method of derivation of \( M_{12} \) is lengthier than in §II.C.

As another remark, it is instructive to recover a known result for the case where \( \mu(x) \) is periodic in one coordinate and does not depend on the other, say \( \mu(x_1, x_2) = \mu(x_1) \). Using (8), (9), (13), and (13) gives
\[
(M_0 - \mathcal{I}) \left( \begin{array}{c} 0 \\ \langle \mu^{-1} \rangle_{1}^{-1} \end{array} \right) = w_0, \quad (M_0 - \mathcal{I}) \left( \begin{array}{c} 0 \\ \langle \mu(x_1) \rangle \end{array} \right) = w_0.
\]
Therefore, by (12) and (13), \( c^2(\kappa_1) = \langle \mu^{-1} \rangle_{1}^{-1} / \langle \rho \rangle \) and \( c^2(\kappa_2) = \langle \mu \rangle / \langle \rho \rangle \) while \( M_{12} = 0 \) by (18) with \( \partial_2 \mu = 0 \).

Finally, we note that, while the above evaluation of quasistatic speed \( c \) is exact, using the same monodromy-matrix approach also provides a closed-form approximation of \( c \). For the isotropic case, it is as follows (see §I.D for more details):
\[
c^2 \approx \frac{1}{2} \left( \left( \langle \mu^{-1} \rangle_{1}^{-1} \right)_2 + \left( \langle \mu \rangle_{2}^{-1} \right)_1 \right).
\]
where \(c(\kappa_i) = c = \text{const. for any } \kappa \) in the isotropic case. The above vectors and matrices are, strictly speaking, of infinite dimension, which needs to be truncated for numerical purposes. In this sense there is no loss of generality in assuming a smooth \(\mu(x)\) in the course of derivations in [1]. Implementation of Eq. (28) consists of two steps.

\[ \hat{\mu}_n(x(i)), n = -N..N \text{ and the } (2N+1) \times (2N+1) \text{ matrices } Q_0(x(i)) \text{ for each } i = 1..N_1\text{, and then use the approximate formula } M_0 = \prod_{i=1}^{N_1} \exp(\Delta_i Q_0(x(i))). \text{ Recall that } \hat{f} \text{ satisfies the chain rule and is exactly equal to } \exp(\Delta_i Q_0) \text{ for } x_1 \in \Delta_i \text{ if } \mu(x) \text{ does not depend on } x_1 \text{ within } \Delta_i. \text{ Therefore the calculation is much simpler in the common case of a piecewise homogeneous unit cell with only a few inclusions of simple shape (see the example below).}

**Step 2.** Solve the system \((M_0 - I)w_1 = iw_0\) for unknown \(w_1\). First remove one zero row and one zero column in the matrix \(M_0 - I\) (see the remark below [10]). Then the vector \(w_1\) is uniquely defined and may be observed by a standard method. Note that only a single component of \(h\) is needed to evaluate \(w_3, w_1\). Finally dividing by \(\langle \rho \rangle\) yields the desired result [28].

As an example, we calculate the effective shear-wave speed \(c\) versus the volume fraction \(f\) of square rods periodically embedded in a matrix material forming a 2D square lattice with translations parallel to the inclusion edges. A high-contrast pair of materials is chosen such as steel (\(\equiv\text{St, with } \rho = 7.8 \times 10^3 \text{ kg m}^{-3}, \mu = 80 \text{ GPa}\)) and epoxy (\(\equiv\text{Ep, with } \rho = 1.14 \times 10^3 \text{ kg m}^{-3}, \mu = 1.48 \text{ GPa}\)). We consider two conjugated St/Ep and Ep/St configurations, where the matrix and rod materials are either St and Ep or Ep and St, respectively. The results are displayed in Fig. 1. The curves \(c_{\text{MM}}(f)\) are computed by the present monodromy-matrix (MM) method, Eq. (28), they are complemented by the approximation [22]. Also shown for comparison are the curves \(c_{\text{PWE}}(f)\) computed from the truncated formula [2] of the conventional PWE method based on a 2D Fourier transform of [3]. Calculations are performed for a different fixed number \(2N + 1 \equiv d\) of the 1D Fourier coefficients of \(\mu(x)\), which implies \(2d \times 2d\) monodromy matrix in [28] and, by contrast, \(d^2 \times d^2\) matrix in the PWE formula [3]. Apart from this advantage of the MM calculation, it is also seen to be remarkably more stable - with a reasonable fit provided already at \(N = 1\). The difference between the MM and PWE numerical curves is especially notable for the case of densely packed steel rods. Interestingly, the MM computation and estimate both predict a steep fall for \(c(f)\) when a small concentration \(1 - f\) of epoxy forms a 'quasi-insulating network'. The PWE fails to capture this important physical feature for reasons described next.

The far superior stability and accuracy of the MM method observed in Fig. 1 can be explained as follows. The PWE formula [3] implies calculating \(M_{11} \approx \sum |g| |g| |g| (|g| + 1)^{-2} + O(d^{-1})\) with bounded coefficients \(B_g\), where \(g\) are the 2D reciprocal lattice vectors (we use here that the components of the vector \(\hat{\partial}_i \mu\) for piecewise constant \(\mu(x)\) are of order \(|g| + 1)^{-1}\), and that the matrix corresponding to \(c_{\text{PWE}}^{-1}\) is close to diagonally-dominant and hence its eigenvalues are of order \(|g|^2\). Thus the accuracy of the PWE method is expected to be of order \(d^{-1}\). In contrast, the accuracy of the MM method, where the 1D Fourier expansion is performed inside a multiplicative integral that is 'close' to exponential, is expected to be on the order \(e^{-d}\). This can be understood from the MM equation (28) [2] where the \(2d \times 2d\) matrix \((M_0 - I)^{-1}\) can be replaced by \(2(M_0 - M_0^{-1})^{-1}\) with eigenvalues of order \(e^{-n}, n = 1..d\).

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8. The subsequent results are equally valid for acoustic waves in fluid-like phononic crystals under the standard interchange of \(\rho\) and \(\mu\) for solids by \(K^{-1}\) and \(\rho^{-1}\) for fluids.