Evaluation of the effective speed of sound in phononic crystals by the monodromy matrix method (L)

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A scheme for evaluating the effective quasistatic speed of sound c in two- and three-dimensional 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 two-dimensional scalar-wave example with extreme behavior. © *2011 Acoustical Society of America*. [DOI: 10.1121/1.3654032]

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I. INTRODUCTION

Long-standing interest in modeling effective acoustic properties of composites with microstructure has substantially intensified with the emerging possibility of designing periodic structures in air[1,2] and in solids[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.[4,5] 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[6] and elastic[7] phononic crystals. At the same time, the PWE calculation is known to face problems when applied to high-contrast composites,[4,5] which are of special interest for applications. Particularly riveting is the case where a soft ingredient is embedded in a way that breaks 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 strong multiple interaction effects, is particularly unsuited for the multiple-scattering approach.[1–3]

The purpose of the present letter is to highlight a new method for evaluating the quasistatic effective sound speed c in two-dimensional (2D) and three-dimensional (3D) phononic crystals. The idea is to recast the wave equation as a first-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 [see Eqs. (12) and (13) for 2D and Eq. (30) for 3D] 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, as demonstrated in the letter for scalar waves in 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 OF 2D ACOUSTIC WAVES

A. Governing equations and problem statement

Consider the scalar wave equation

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

for time-harmonic shear displacement $v(\mathbf{x},t) = v(\mathbf{x})e^{-i\omega t}$ in a 2D solid continuum with $\mathbf{T}$-periodic density $\rho(\mathbf{x})$ and shear coefficient $\mu(\mathbf{x})$. The subsequent results are equally valid for waves in fluid-like phononic crystals under the standard interchange of ρ and μ for solids by K^{-1} and ρ^{-1} for fluids. Assume a square unit cell $\mathbf{T} = \{\sum_i t_i \mathbf{a}_i\} = [0,1]^2$ with unit translation vectors $\mathbf{a}_1 \perp \mathbf{a}_2$ taken as the basis for $\mathbf{x} = \sum_i x_i \mathbf{a}_i$. Imposing the Floquet condition $v(\mathbf{x}) = u(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}$, where $u(\mathbf{x})$ is periodic and $\mathbf{k} = k\boldsymbol{\kappa}$ ($|\boldsymbol{\kappa}| = 1$), Eq. (1) becomes

$$\begin{aligned}(\mathcal{C}_0 + \mathcal{C}_1 + \mathcal{C}_2)u = \rho\omega^2 u \quad \text{with} \quad \mathcal{C}_0 u = -\nabla(\mu\nabla u)\\ \mathcal{C}_1 u = -i\mathbf{k}\cdot(\mu\nabla u + \nabla(\mu u)), \quad \mathcal{C}_2 u = k^2\mu u.\end{aligned} \tag{2}$$

Regular perturbation theory applied to Eq. (2) yields the effective speed $c(\boldsymbol{\kappa}) = \lim_{\omega,k\to 0} \omega(\mathbf{k})/k$ in the following form:[8]

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$$c^2(\boldsymbol{\kappa}) = \mu_{\text{eff}}(\boldsymbol{\kappa})/\langle\rho\rangle, \quad \mu_{\text{eff}}(\boldsymbol{\kappa}) = \langle\mu\rangle - M(\boldsymbol{\kappa}) \quad \text{with}$$
$$M(\boldsymbol{\kappa}) = \sum_{i,j=1}^{2} M_{ij}\kappa_i\kappa_j, \quad M_{ij} = \left(\mathcal{C}_0^{-1}\partial_i\mu, \partial_j\mu\right) = M_{ji}, \quad (3)$$

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

$$\langle f\rangle \equiv \int_{\mathbf{T}} f(\mathbf{x})\mathrm{d}\mathbf{x} \left(= \left\langle\langle f\rangle_1\right\rangle_2, \quad \langle f\rangle_i \equiv \int_0^1 f(\mathbf{x})\mathrm{d}x_i\right), \quad (4)$$

and $(\cdot,\cdot)$ denotes the scalar product in $L^2(\mathbf{T})$ so that $(f,h) = \langle fh^*\rangle$ [the asterisk (*) means complex conjugation]. The difficulty with Eq. (3) is that it involves the inverse of a partial differential operator $\mathcal{C}_0$. One solution is to apply a double Fourier expansion to $\mathcal{C}_0^{-1}$ and $\partial_i\mu$ in Eq. (3). This leads to the PWE formula for the effective speed,[6] which is expressed via infinite vectors and the inverse of the infinite matrix of Fourier coefficients of $\mu(\mathbf{x})$. 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 Sec. IV). An alternative "brute force" procedure of the scaling approach is to numerically solve the partial differential equation $\mathcal{C}_0 h = \partial_i\mu$ for the 1-periodic function $h(\mathbf{x})$ (e.g., via the boundary integral method).[9]

The new approach proposed here leads to a more efficient 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" Eq. (3). This is convenient for deriving $c(\boldsymbol{\kappa})$ in the principal directions $\boldsymbol{\kappa} \parallel \mathbf{a}_{1,2}$, see Sec. II B. The second method is more closely related to the conventional PWE and scaling approaches in that it also starts from Eq. (3) but treats it differently, namely, the equation $\mathcal{C}_0 h = \partial_i\mu$ is cast in ODS form and analytically integrated in one coordinate. This is basically equivalent to the former method, but enables an easier derivation of the off-diagonal component M_{12} for the anisotropic case, see Sec. II C.

B. Wave speed in the principal directions

The wave equation (1) may be recast as

$$\boldsymbol{\eta}' = \mathcal{Q}\boldsymbol{\eta} \text{ with } \mathcal{A} = -\partial_2(\mu\partial_2)$$
$$\mathcal{Q} = \begin{pmatrix} 0 & \mu^{-1} \\ \mathcal{A} - \rho\omega^2 & 0 \end{pmatrix}, \quad \boldsymbol{\eta}(\mathbf{x}) = \begin{pmatrix} v \\ \mu v' \end{pmatrix}, \quad (5)$$

where the prime ($'$) stands for ∂_1. The solution to Eq. (5) for initial data $\boldsymbol{\eta}(0,x_2) \equiv \boldsymbol{\eta}(0,\cdot)$ at $x_1 = 0$ is

$$\boldsymbol{\eta}(x_1,\cdot) = \mathcal{M}[x_1,0]\boldsymbol{\eta}(0,\cdot) \quad \text{with}$$
$$\mathcal{M}[a,b] = \widehat{\int_b^a}(\mathcal{I} + \mathcal{Q}\mathrm{d}x_1). \quad (6)$$

The operator $\mathcal{M}[x_1,0]$ is formally the matricant, or propagator, of Eq. (6) defined through the multiplicative integral $\widehat{\int}$ (with $\mathcal{I}$ denoting the identity operator). It is assumed for the moment that $\rho(\mathbf{x})$ and $\mu(\mathbf{x})$ are smooth to ensure the existence of $\mathcal{M}$. The matricant over a period, $\mathcal{M}[1,0]$, is called the monodromy matrix.

Assume the Floquet condition with the wave vector $\mathbf{k} = (k_1\ 0)^{\mathrm{T}}$ so that $v(\mathbf{x}) = u(\mathbf{x})e^{ik_1x_1}$ and $\boldsymbol{\eta}(1,\cdot) = \boldsymbol{\eta}(0,\cdot)e^{ik_1}$ By Eq. $(6)_1$, this implies the eigenproblem

$$\mathcal{M}[1,0]\ \mathbf{w}(k_1) = e^{ik_1}\ \mathbf{w}(k_1). \quad (7)$$

Equation (7) defines $k_1 = k_1(\omega)$ (since $\mathcal{M}$ depends on ω) and hence $\omega = \omega(k_1)$, where ω^2 is the eigenvalue of Eq. (1) with $v(\mathbf{x}) = u(\mathbf{x})e^{ik_1x_1}$. The effective speed $c(\mathbf{a}_1) = \lim_{\omega,k_1\to 0}\omega/k_1$ can therefore be determined by applying perturbation theory to Eq. (7) as $\omega, k_1 \to 0$. The asymptotic form[10] of $\mathcal{M}[1,0]$ follows from definitions (5) and $(6)_2$ as

$$\mathcal{M}[1,0] = \mathcal{M}_0 + \omega^2\mathcal{M}_1 + O(\omega^4) \text{ where}$$
$$\mathcal{M}_0 \equiv \mathcal{M}_0[1,0], \quad \mathcal{M}_0[a,b] = \widehat{\int_b^a}(\mathcal{I} + \mathcal{Q}_0\mathrm{d}x_1) \quad \text{with}$$
$$\mathcal{Q}_0 \equiv \mathcal{Q}_{\omega=0} = \begin{pmatrix} 0 & \mu^{-1} \\ \mathcal{A} & 0 \end{pmatrix},$$
$$\mathcal{M}_1 = \int_0^1 \mathcal{M}_0[1,x_1]\begin{pmatrix} 0 & 0 \\ -\rho & 0 \end{pmatrix}\mathcal{M}_0[x_1,0]\mathrm{d}x_1. \quad (8)$$

Note the identities $\mathcal{Q}_0\mathbf{w}_0 = \mathbf{0}$, $\mathcal{Q}_0^+\tilde{\mathbf{w}}_0 = \mathbf{0}$ [where the plus sign ($^+$) is Hermitian conjugation] and hence

$$\mathcal{M}_0[a,b]\mathbf{w}_0 = \mathbf{w}_0, \quad \mathcal{M}_0^+[a,b]\tilde{\mathbf{w}}_0 = \tilde{\mathbf{w}}_0\ (\forall a,b)$$
$$\text{for} \quad \mathbf{w}_0(x_2) = (1\ 0)^{\mathrm{T}}, \quad \tilde{\mathbf{w}}_0(x_2) = (0\ 1)^{\mathrm{T}}. \quad (9)$$

By Eq. $(9)_1$ $\mathbf{w}_0$ is an eigenvector of $\mathcal{M}_0$ with the eigenvalue 1, and it can be shown to be a single eigenvector. Therefore $\mathbf{w}(k_1) = \mathbf{w}_0 + k_1\mathbf{w}_1 + k_1^2\mathbf{w}_2 + O(k_1^3)$ and $\omega = ck_1 + O(k_1^2)$. Insert these expansions along with $(8)_1$ in Eq. (7) and collect the first-order terms in k_1 to obtain

$$\mathcal{M}_0\mathbf{w}_1 = \mathbf{w}_1 + i\mathbf{w}_0 \Rightarrow \mathbf{w}_1 = i(\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0. \quad (10)$$

According to Eq. (9), $M_0 - \mathcal{I}$ has no inverse but is a one-to-one mapping from some subspace orthogonal to $\mathbf{w}_0$ onto the subspace orthogonal $\tilde{\mathbf{w}}_0$; hence, $\mathbf{w}_1$ exists and $\tilde{\mathbf{w}}_0\cdot\mathbf{w}_1$ is uniquely defined. The terms of second order in k_1 in Eq. (7) then imply

$$\mathcal{M}_0\mathbf{w}_2 + c^2\mathcal{M}_1\mathbf{w}_0 = -\frac{1}{2}\mathbf{w}_0 + i\mathbf{w}_1 + \mathbf{w}_2. \quad (11)$$

Scalar multiplication on both sides by $\tilde{\mathbf{w}}_0$ leads, with account for Eqs. (9) and $(8)_4$, to $c^2\langle\rho\rangle = -i\langle\tilde{\mathbf{w}}_0\cdot\mathbf{w}_1\rangle_2$, hence by Eq. $(10)_2$,

$$c^2(\mathbf{a}_1) = \langle\rho\rangle^{-1}\left\langle\tilde{\mathbf{w}}_0\cdot(\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0\right\rangle_2, \quad (12)$$

where the notation $\langle\cdot\rangle_2$ is explained in Eq. (4) and $\cdot$ is a scalar product in vector space. Interchanging variables $x_1 \rightleftarrows x_2$ in the above-mentioned derivation yields a similar result for $c(\mathbf{a}_2)$ as follows:

$$
\begin{aligned}
&c^2(\mathbf{a}_2) = \langle\rho\rangle^{-1}\left\langle \tilde{\mathbf{w}}_0 \cdot (\widetilde{\mathcal{M}}_0 - \mathcal{I})^{-1}\mathbf{w}_0 \right\rangle_1 \text{ where} \\
&\widetilde{\mathcal{M}}_0 = \widehat{\int_0^1} (\mathcal{I} + \tilde{\mathcal{Q}}_0 \mathrm{d}x_2), \\
&\tilde{\mathcal{Q}}_0 = \begin{pmatrix} 0 & \mu^{-1} \\ \tilde{\mathcal{A}} & 0 \end{pmatrix}, \quad \tilde{\mathcal{A}} = -\partial_1(\mu\partial_1).
\end{aligned} \tag{13}
$$

The result for a rectangular lattice readily follows by rescaling of the coordinates x_i; a similar formula for an oblique lattice can be obtained via the coordinate transformation from the oblique to orthogonal basis.

Even μ. For an even function $\mu(x_1, x_2) = \mu(-x_1, x_2)$ formula (12) can be simplified. The chain rule for the multiplicative integral (6) and the identity (9) yield

$$
\begin{aligned}
(\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0 &= (\mathcal{M}_0[1, \tfrac{1}{2}]\mathcal{M}_0[\tfrac{1}{2}, 0] - \mathcal{I})^{-1}\mathbf{w}_0 \\
&= (\mathcal{M}_0[\tfrac{1}{2}, 0] - \mathcal{M}_0^{-1}[1, \tfrac{1}{2}])^{-1}\mathbf{w}_0.
\end{aligned} \tag{14}
$$

Denoting

$$
\mathcal{M}_0[\tfrac{1}{2}, 0] = \widehat{\int_0^{1/2}} (\mathcal{I} + \mathcal{Q}_0 \mathrm{d}x_1) \equiv \begin{pmatrix} \mathcal{M}_{01} & \mathcal{M}_{02} \\ \mathcal{M}_{03} & \mathcal{M}_{04} \end{pmatrix} \tag{15}
$$

and using the symmetry of μ leads to

$$
\mathcal{M}_0^{-1}[1, \tfrac{1}{2}] = \widehat{\int_0^{1/2}} (\mathcal{I} - \mathcal{Q}_0 \mathrm{d}x_1) = \begin{pmatrix} \mathcal{M}_{01} & -\mathcal{M}_{02} \\ -\mathcal{M}_{03} & \mathcal{M}_{04} \end{pmatrix}. \tag{16}
$$

Combining Eqs. (14)–(16) with Eq. (12) then gives

$$
c^2(\mathbf{a}_1) = \frac{1}{2}\langle\rho\rangle^{-1}\left\langle \mathcal{M}_{02}^{-1} e \right\rangle_2, \quad e(x_2) \equiv 1. \tag{17}
$$

C. The full matrix M_{ij}

The anisotropy of the effective speed $c(\boldsymbol{\kappa})$, i.e., its dependence on the wave normal $\boldsymbol{\kappa} \equiv \mathbf{k}/k$, is determined by the quadratic form $M(\boldsymbol{\kappa}) = \sum_{i,j=1}^2 M_{ij}\kappa_i\kappa_j$ [see Eq. (3)], and represented by the ellipse of (squared) slowness $c^{-2}(\boldsymbol{\kappa})$. Equations (12) and $(13)_1$, which define $c(\mathbf{a}_i)$ and so M_{ii}, suffice for the case where $\mathbf{T}$ is rectangular and $\mu(\mathbf{x})$ is even in (at least) one of x_i so that the effective-slowness ellipse is $c^{-2}(\boldsymbol{\kappa}) = \sum_{i=1,2} c^{-2}(\mathbf{a}_i)\kappa_i^2$ with the principal axes parallel to $\mathbf{a}_1 \perp \mathbf{a}_2$. Otherwise $c(\boldsymbol{\kappa})$ for arbitrary $\boldsymbol{\kappa}$ requires finding the off-diagonal component M_{12}. For this purpose, with reference to Eq. (3), consider the equation

$$
\mathcal{C}_0 h = \partial_1\mu \tag{18}
$$

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

$$
\boldsymbol{\xi}' = \mathcal{Q}_0\boldsymbol{\xi} \quad \text{where} \quad \boldsymbol{\xi} = \begin{pmatrix} h + x_1 \\ \mu(h' + 1) \end{pmatrix} \tag{19}
$$

and $\mathcal{Q}_0$ is given in Eq. $(8)_3$. The general solution to Eq. (19) is

$$
\boldsymbol{\xi}(x_1, \cdot) = \mathcal{M}_0[x_1, 0]\boldsymbol{\xi}(0, \cdot), \tag{20}
$$

where $\mathcal{M}_0[x_1, 0]$ is defined in Eq. $(8)_2$, and $\boldsymbol{\xi}(0, \cdot)$ is the initial data at $x_1 = 0$. The periodicity of h implies $\boldsymbol{\xi}(1, \cdot) = \boldsymbol{\xi}(0, \cdot) + \mathbf{w}_0$, while $\boldsymbol{\xi}(1, \cdot) = \mathcal{M}_0\boldsymbol{\xi}(0, \cdot)$ by Eq. (16). Hence $\boldsymbol{\xi}(0, \cdot) = (\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0$ and so Eq. (18) is solved by

$$
\boldsymbol{\xi}(x_1, \cdot) = \mathcal{M}_0[x_1, 0](\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0. \tag{21}
$$

Substituting Eq. (21) into the definition of M_{12} in Eq. (3) yields

$$
\begin{aligned}
M_{12} &= (\mathcal{C}_0^{-1}\partial_1\mu, \partial_2\mu) = \langle h\partial_2\mu\rangle = \langle \partial_2\mu\mathbf{w}_0 \cdot \boldsymbol{\xi}\rangle \\
&= \left\langle \partial_2\mu\mathbf{w}_0 \cdot \mathcal{M}_0[x_1, 0](\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0 \right\rangle.
\end{aligned} \tag{22}
$$

Note that the formula (22) for M_{12} requires more computation than the formulas (12) and $(13)_1$ for M_{ii}. Interestingly, if the unit cell $\mathbf{T}$ is square, then, for an arbitrary (periodic) $\mu(\mathbf{x})$, Eq. (22) can be circumvented by using the identity $M_{12} = (\widetilde{M}_{11} - \widetilde{M}_{22})/2$, where $\widetilde{M}_{ii}$ follows from Eqs. (12) and $(13)_1$ applied to the square lattice obtained from the given one by turning it 45°.

D. Discussion

The two lines of attack outlined in Sec. II A are equivalent in that the formula (12) for the effective speed $c(\mathbf{a}_1)$ in the principal direction can also be inferred from Eq. (3). Inserting the solution (21) of Eq. (18) defines the component M_{11} as

$$
M_{11} = (\mathcal{C}_0^{-1}\partial_1\mu, \partial_1\mu) = \langle h\mu'\rangle = \langle \mu'\mathbf{w}_0 \cdot \boldsymbol{\xi}\rangle - \langle x_1\mu'\rangle. \tag{23}
$$

Integrating by parts each term in the last identity and using the periodicity of $\mu(\mathbf{x})$ along with Eqs. $(8)_3$, (9), (19)–(21) [see also the notation (4)] yields

$$
\begin{aligned}
\langle \mu'\mathbf{w}_0 \cdot \boldsymbol{\xi}\rangle &= -\langle \mu\mathbf{w}_0 \cdot \boldsymbol{\xi}'\rangle + \langle \mu(1, x_2)\mathbf{w}_0 \cdot \boldsymbol{\xi}(x_2)\rangle_2 \\
&\quad - \langle \mu(0, x_2)\mathbf{w}_0 \cdot \boldsymbol{\xi}(x_2)\rangle_2 \\
&= -\langle \mu\mathbf{w}_0 \cdot \mathcal{Q}_0\boldsymbol{\xi}\rangle + \langle \mu(0, x_2)\mathbf{w}_0 \cdot (\boldsymbol{\xi}(1, x_2) \\
&\quad - \boldsymbol{\xi}(0, x_2))\rangle_2 \\
&= -\langle \tilde{\mathbf{w}}_0 \cdot \boldsymbol{\xi}\rangle + \langle \mu(0, x_2)\mathbf{w}_0 \cdot (\mathcal{M}_0 - \mathcal{I})\boldsymbol{\xi}(0, x_2))\rangle_2 \\
&= -\langle \tilde{\mathbf{w}}_0 \cdot \mathcal{M}_0[x_1, 0](\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0\rangle + \langle \mu(0, x_2)\rangle_2 \\
&= -\langle \tilde{\mathbf{w}}_0 \cdot (\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0\rangle + \langle \mu(0, x_2)\rangle_2 \\
&= -\langle \tilde{\mathbf{w}}_0 \cdot (\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0\rangle_2 + \langle \mu(0, x_2)\rangle_2, \\
&\quad - \langle x_1\mu'\rangle = \langle\mu\rangle - \langle \mu(1, x_2)\rangle_2 \\
&= \langle\mu\rangle - \langle \mu(0, x_2)\rangle_2.
\end{aligned} \tag{24}
$$

Thus, $M_{11} = \langle\mu\rangle - \langle \tilde{\mathbf{w}}_0 \cdot (\mathcal{M}_0 - \mathcal{I})^{-1}\mathbf{w}_0\rangle_2$, which leads to Eq. (12). Note that Eq. (22) is also obtainable via the monodromy matrix of the wave equation (1) (the approach of Sec. II B) with $v(\mathbf{x}) = u(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}$ and $\mathbf{k} \nparallel \mathbf{a}_i$, but this method of derivation of M_{12} is lengthier than in Sec. II C.

As another remark, it is instructive to recover a known result for the case where $\mu(\mathbf{x})$ is periodic in one coordinate and does not depend on the other, say $\mu(x_1,x_2)=\mu(x_1)$. Using Eqs. (8)$_2$, (8)$_3$, and (13)$_3$ gives

$$(\mathcal{M}_0-\mathcal{I})\begin{pmatrix}0\\ \langle\mu^{-1}\rangle_1^{-1}\end{pmatrix}=\mathbf{w}_0,$$
$$(\widetilde{\mathcal{M}}_0-\mathcal{I})\begin{pmatrix}0\\ \mu(x_1)\end{pmatrix}=\mathbf{w}_0. \tag{25}$$

Therefore, by Eqs. (12) and (13)$_1$, $c^2(\mathbf{a}_1)=\langle\mu^{-1}\rangle_1^{-1}/\langle\rho\rangle$ and $c^2(\mathbf{a}_2)=\langle\mu\rangle_1/\langle\rho\rangle$ while $M_{12}=0$ by Eq. (22) with $\partial_2\mu=0$.

Finally, we note that, while the above-presented 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:[8]

$$c^2\approx\frac{1}{2\langle\rho\rangle}\left(\left\langle\left\langle\mu^{-1}\right\rangle_1^{-1}\right\rangle_2+\left\langle\langle\mu\rangle_2^{-1}\right\rangle_1^{-1}\right). \tag{26}$$

III. EFFECTIVE SPEEDS IN PRINCIPAL DIRECTIONS FOR 3D ELASTIC WAVES

The equation for time-harmonic elastic wave motion $\mathbf{v}(\mathbf{x},t)=\mathbf{v}(\mathbf{x})e^{-i\omega t}$ is, with repeated suffices summed,

$$-\partial_j(c_{ijkl}\partial_l v_k)=\rho\omega^2 v_i\quad(i,j,k,l=1,2,3), \tag{27}$$

where density $\rho(\mathbf{x})$ and compliances $c_{ijkl}(\mathbf{x})$ are $\mathbf{T}$-periodic in a 3D periodic medium. Assume a cubic unit cell $\mathbf{T}=\{\sum_i t_i\mathbf{a}_i\}=[0,1]^3$ and refer the components x_i, v_i, and c_{ijkl} to the orthogonal basis formed by the translation vectors $\mathbf{a}_i$. Impose the condition $\mathbf{v}(\mathbf{x})=\mathbf{u}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}$ with periodic $\mathbf{u}(\mathbf{x})=(u_i)$ and take $\mathbf{k}$ parallel to one of the $\mathbf{a}_i$, e.g., to $\mathbf{a}_1$. Equation (27) may be rewritten in the form

$$\boldsymbol{\eta}'=\mathcal{Q}\boldsymbol{\eta}\ \text{with}\ \boldsymbol{\eta}(\mathbf{x})=\begin{pmatrix}(u_i)\\(c_{i1kl}\partial_l u_k)\end{pmatrix},$$
$$\mathcal{Q}=\begin{pmatrix}-\mathcal{C}^{-1}\mathcal{A}_1 & \mathcal{C}^{-1}\\ -\omega^2\rho\delta_{ij}+\mathcal{A}_2-\mathcal{A}_1^{+}\mathcal{C}^{-1}\mathcal{A}_1 & \mathcal{A}_1^{+}\mathcal{C}^{-1}\end{pmatrix}, \tag{28}$$

where the matrix operators $\mathcal{A}_1$ and self-adjoint $\mathcal{A}_2,\mathcal{C}$ are

$$\mathcal{C}=(c_{i1k1}),\quad \mathcal{A}_1(u_i)=(c_{i1ka}\partial_a u_k),$$
$$\mathcal{A}_2(u_i)=-(\partial_a(c_{iakb}\partial_b u_k))\quad\text{with}\quad a,b=2,3. \tag{29}$$

Like in the 2D case, denote the monodromy matrix for Eq. (28) at $\omega=0$ by $\mathcal{M}_0=\widehat{\int}_0^1(\mathcal{I}+\mathcal{Q}_0dx_1)$, where $\mathcal{Q}_0=\mathcal{Q}_{\omega=0}$, and also introduce the 6×3 matrices $\mathbf{W}_0=(\delta_{ij}\ \mathbf{0})^{\mathrm{T}}$ and $\widetilde{\mathbf{W}}_0=(\mathbf{0}\ \delta_{ij})^{\mathrm{T}}$. Reasoning similar to that in Sec. II C leads us to the conclusion that the effective speeds $c_\alpha(\mathbf{a}_1)=\lim_{\omega,k_1\to0}\omega/k_1$ $(\alpha=1,2,3)$ of the three waves with $\mathbf{k}\equiv k\boldsymbol{\kappa}$ parallel to $\mathbf{a}_1$ are the eigenvalues of the 3×3 matrix

$$\left\langle\left\langle\widetilde{\mathbf{W}}_0^{+}(\mathcal{M}_0-\mathcal{I})^{-1}\mathbf{W}_0\right\rangle_2\right\rangle_3\quad(\text{with }\langle\cdot\rangle_i\equiv(4)). \tag{30}$$

IV. NUMERICAL IMPLEMENTATION

There are several ways to use the above-presented analytical results for calculating the effective speed. One approach is to transform to Fourier space with respect to coordinate(s) other than the coordinate of integration in the monodromy matrix. Consider the 2D case and apply the Fourier expansion $f(x_1,x_2)=\sum_{n\in\mathbb{Z}}\widehat{f}_n(x_1)e^{2\pi inx_2}$ in x_2 for the functions $f=\mu$ and μ^{-1}. Then the operator of multiplying by the function $\mu^{-1}(x_1,\cdot)$ and the differential operator $\mathcal{A}(x_1)=-\partial_2(\mu(x_1,\cdot)\partial_2)$ become matrices

$$\mu^{-1}\mapsto\boldsymbol{\mu}^{-1}(x_1)=(\widehat{\mu^{-1}}_{n-m})=(\widehat{\mu}_{n-m})^{-1}$$
$$\mathcal{A}\mapsto\mathbf{A}(x_1)=4\pi^2(nm\widehat{\mu}_{n-m}),\quad n,m\in\mathbb{Z} \tag{31}$$

and Eq. (12) reduces to the following form:

$$c^2(\mathbf{a}_1)=\langle\rho\rangle^{-1}\tilde{\mathbf{w}}_{\hat{0}}\cdot(\mathbf{M}_0-\mathbf{I})^{-1}\mathbf{w}_{\hat{0}}\quad\text{with}$$
$$\mathbf{M}_0=\widehat{\int}_0^1(\mathbf{I}+\mathbf{Q}_0dx_1),\quad \mathbf{Q}_0(x_1)=\begin{pmatrix}\mathbf{0}&\boldsymbol{\mu}^{-1}\\ \mathbf{A}&\mathbf{0}\end{pmatrix},$$
$$\tilde{\mathbf{w}}_{\hat{0}}=(\mathbf{0}\ \delta_{0n})^{\mathrm{T}},\quad \mathbf{w}_{\hat{0}}=(\delta_{0n}\ \mathbf{0})^{\mathrm{T}}, \tag{32}$$

where $c(\boldsymbol{\kappa})=c=\text{const}$ for any $\boldsymbol{\kappa}$ in the isotropic case. The above-mentioned 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 $\mu(\mathbf{x})$ in the course of derivations in Sec. II. Implementation of Eq. (32)$_1$ consists of two steps.

Step 1. Calculate the multiplicative integral (32)$_1$ defining $\mathbf{M}_0$. For an arbitrary $\mu(\mathbf{x})$, one way is to use a discretization scheme. Divide the segment $x_1\in[0,1]$ into N_1 intervals $\Delta_i\equiv[x_1^{(i)},x_1^{(i+1)})$, $i=1,\dots,N_1$, of small enough length. Calculate $2N+1$ Fourier coefficients $\hat{\mu}_n(x_1^{(i)})$, $n=-N,\dots,N$ and the $(2N+1)\times(2N+1)$ matrices $\mathbf{Q}_0(x_1^{(i)})$ for each $i=1,\dots,N_1$, and then use the approximate formula $\mathbf{M}_0=\Pi_{i=N_1}^{1}\exp[|\Delta_i|\hat{\mathbf{Q}}_0(x_1^{(i)})]$. Recall that $\widehat{\int}$ satisfies the chain rule and $\widehat{\int}_b^a=\exp[(a-b)\mathbf{Q}_0]$ for $a,b\in\Delta$ if $\mu(\mathbf{x})$ does not depend on x_1 within Δ. 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 to follow).

Step 2. Solve the system $(\mathbf{M}_0-\mathbf{I})\mathbf{w}_{\hat{1}}=i\mathbf{w}_{\hat{0}}$ for unknown $\mathbf{w}_{\hat{1}}$. First remove one zero row and one zero column in the matrix $\mathbf{M}_0-\mathbf{I}$ [see the remark following Eq. (10)]. Then the vector $\mathbf{w}_{\hat{1}}$ is uniquely defined and may be found by any standard method. Note that only a single component of $\mathbf{w}_{\hat{1}}$ is needed to evaluate $\tilde{\mathbf{w}}_{\hat{0}}\cdot\mathbf{w}_{\hat{1}}$. Finally dividing by $\langle\rho\rangle$ yields the desired result (32)$_1$. Note that the case of even μ admits a simpler formula (17), which implies

$$c^2(\mathbf{a}_1)=\frac{1}{2}\langle\rho\rangle^{-1}(\delta_{n0})\cdot\mathbf{m}^{-1}(\delta_{n0}), \tag{33}$$

where $\mathbf{m}$ is the upper right block of the matrix $\mathbf{M}_0[\frac{1}{2},0]=\widehat{\int}_0^{1/2}(\mathbf{I}+\mathbf{Q}_0dx_1)$.

As an example, we calculate the effective shear-wave speed c versus the volume fraction f of square rods

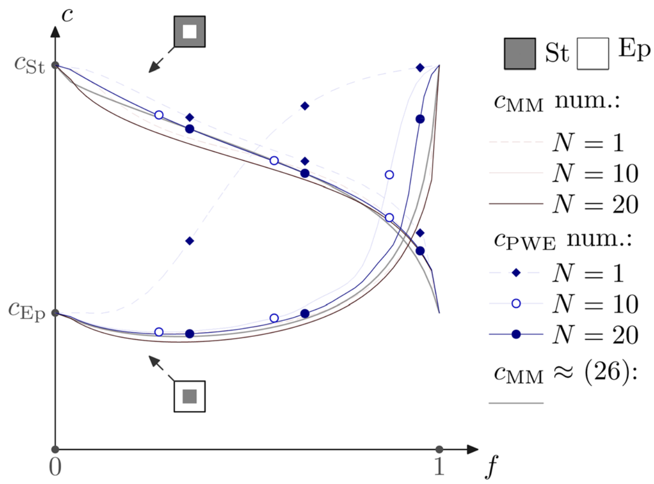

FIG. 1. (Color online) Effective speed c versus concentration f of square rods for 2D St/Ep and Ep/St lattices (see details in the text).

periodically embedded in a matrix material to form a 2D square lattice with translations parallel to the inclusion edges. A high-contrast pair of materials is chosen such as steel ($\equiv$St, with $\rho = 7.8 \times 10^3$ kg/m^3, $\mu = 80$ GPa) and epoxy ($\equiv$Ep, with $\rho = 1.14 \times 10^3$ kg/m^3, $\mu = 1.48$ 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 $c_{MM}(f)$ are computed by the present monodromy-matrix (MM) method, Eq. (33); they are complemented by the approximation (26). Also shown for comparison are the curves $c_{PWE}(f)$ computed from the truncated formula[6] of the conventional PWE method based on a 2D Fourier transform of Eq. (3). Calculations are performed for a different fixed number $2N + 1 \equiv d$ of the one-dimensional (1D) Fourier coefficients of $\mu(\mathbf{x})$, which implies a $d \times d$ matrix $\mathbf{m}$ in Eq. (33) and, by contrast, a $d^2 \times d^2$ matrix in the PWE formula.[6] 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 demonstrated in Fig. 1 can be explained as follows. The PWE formula[6] implies calculating $M_{11} \approx \sum_{|\mathbf{g}|<d} B_{\mathbf{g}} |\mathbf{g}|^{-2} (|g_2| + 1)^{-2} + O(d^{-1})$ with bounded coefficients $B_{\mathbf{g}}$, where $\mathbf{g}$ are the 2D reciprocal lattice vectors [we use here that the components of the vector $\widehat{\partial_1 \mu}$ for piecewise constant $\mu(\mathbf{x})$ are of order $(|g_2| + 1)^{-1}$, and that the matrix corresponding to $\mathcal{C}_0^{-1}$ is close to diagonally dominant and hence its eigenvalues are of order $|\mathbf{g}|^{-2}$]. 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 $(32)_1$, where the $2d \times 2d$ matrix $(\mathbf{M}_0 - \mathbf{I})^{-1}$ can be replaced by $2(\mathbf{M}_0 - \mathbf{M}_0^{-1})^{-1}$ with eigenvalues of order $e^{-n}, n = 1, \ldots, d$.

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