Weak forms for Bloch eigenproblems

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July 27, 2023

Contents

1 Notation

In this document, the following notation is observed:

ω temporal frequency

κ wave number (spatial frequency)

ι ("iota") the imaginary unit

i, j, k, l, m subscripts indicating vector/tensor components

Bold symbols indicate vectors, e.g. $\boldsymbol{x}$ is the position vector with components x_i.

2 Problems considered

2.1 Scalar Helmholtz equation

Eigenproblem:

$$\nabla \cdot (\boldsymbol{E}(\boldsymbol{x})\nabla w(\boldsymbol{x},t)) = \rho(\boldsymbol{x})\ddot{w}(\boldsymbol{x},t)$$
$$(E_{ij}(\boldsymbol{x})w_{,j}(\boldsymbol{x},t))_{,i} = \rho(\boldsymbol{x})\ddot{w}(\boldsymbol{x},t)$$
$$w(\boldsymbol{x},t) = u(\boldsymbol{x})e^{-\iota\omega t}$$
$$(E_{ij}(\boldsymbol{x})u_{,j}(\boldsymbol{x}))_{,i}\, e^{-\iota\omega t} = -\,\omega^2\rho(\boldsymbol{x})u(\boldsymbol{x})e^{-\iota\omega t}$$
$$(E_{ij}(\boldsymbol{x})u_{,j}(\boldsymbol{x}))_{,i} = -\,\omega^2\rho(\boldsymbol{x})u(\boldsymbol{x}) \tag{1}$$

2.2 Elasticity equation

Eigenproblem:

$$\nabla \cdot (\boldsymbol{E}(\boldsymbol{x})\nabla_s \boldsymbol{w}(\boldsymbol{x},t)) = \rho(\boldsymbol{x})\ddot{\boldsymbol{w}}(\boldsymbol{x},t)$$
$$\left(E_{ijkl}(\boldsymbol{x})\frac{1}{2}\left(w_{k,l}(\boldsymbol{x},t) + w_{l,k}(\boldsymbol{x},t)\right)\right)_{,i} = \rho(\boldsymbol{x})\ddot{w}_j(\boldsymbol{x},t)$$
$$w_j(\boldsymbol{x},t) = u_j(\boldsymbol{x})e^{-\iota\omega t}$$
$$\left(E_{ijkl}(\boldsymbol{x})\frac{1}{2}\left(u_{k,l}(\boldsymbol{x}) + u_{l,k}(\boldsymbol{x})\right)\right)_{,i} e^{-\iota\omega t} = -\,\omega^2\rho(\boldsymbol{x})u_j(\boldsymbol{x})e^{-\iota\omega t}$$
$$\left(E_{ijkl}(\boldsymbol{x})\frac{1}{2}\left(u_{k,l}(\boldsymbol{x}) + u_{l,k}(\boldsymbol{x})\right)\right)_{,i} = -\,\omega^2\rho(\boldsymbol{x})u_j(\boldsymbol{x}) \tag{2}$$

2.3 Bloch ansatz

Bloch waves have the form

$$u(\boldsymbol{x}) = \tilde{u}(\boldsymbol{x})e^{-\iota\boldsymbol{\kappa}\cdot\boldsymbol{x}}\,, \tag{3}$$

where $\tilde{u}(\boldsymbol{x})$ is a function that is periodic on the unit cell.

3 Direct $(\boldsymbol{\kappa}(\omega))$

In the direct formulation (see Collet et al., 2011), we prescribe the temporal frequency ω and wave direction $\boldsymbol{\phi}$ and compute the wavevector magnitudes as the eigenvalues. The periodic functions $\tilde{u}(\boldsymbol{x})$ are the eigenfunctions.
TODO: write me

4 Indirect $(\omega(\boldsymbol{\kappa}))$, untransformed

In the untransformed indirect formulation, we prescribe the wavevector through Floquet-periodic boundary conditions and solve for the temporal frequencies ω as eigenvalues. The Floquet-periodic displacement fields $u(\boldsymbol{x})$ are the corresponding eigenfunctions.

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5 Indirect ($\omega(\boldsymbol{\kappa})$), with Bloch transformation

In the transformed indirect formulation, the Bloch ansatz is used to transform the equations of motion in terms of the periodic function $\tilde{u}(\boldsymbol{x})$. The wavevector $\boldsymbol{\kappa}$ is prescribed through additional terms that arise in the strong form of the problem, and the temporal frequency ω is solved as the eigenvalue. The periodic functions $\tilde{u}(\boldsymbol{x})$ are the corresponding eigenfunctions.

5.1 Scalar Helmholtz equation

5.1.1 Derivation of transformed strong form

Consider the eigenproblem (1) and insert the Bloch ansatz (3):

$$\left(E_{ij}(\boldsymbol{x}) \left[\tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k} \right]_{,j} \right)_{,i} = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k}$$

$$\left(E_{ij}(\boldsymbol{x}) \left[\tilde{u}_{,j}(\boldsymbol{x})e^{-\iota \kappa_k x_k} + \tilde{u}(\boldsymbol{x})(e^{-\iota \kappa_k x_k})_{,j} \right] \right)_{,i} = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k}$$

$$\left(E_{ij}(\boldsymbol{x}) \left[\tilde{u}_{,j}(\boldsymbol{x})e^{-\iota \kappa_k x_k} + \tilde{u}(\boldsymbol{x})e^{-\iota \kappa_m x_m}(-\iota \kappa_k \delta_{kj}) \right] \right)_{,i} = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k}$$

$$\left(E_{ij}(\boldsymbol{x}) \left[\tilde{u}_{,j}(\boldsymbol{x})e^{-\iota \kappa_k x_k} - \iota \kappa_j \tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k} \right] \right)_{,i} = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k}$$

$$\left(E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x})e^{-\iota \kappa_k x_k} - \iota E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k} \right)_{,i} = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k}$$

$$\left(E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x})e^{-\iota \kappa_k x_k} \right)_{,i} - \iota \left(E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k} \right)_{,i} = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k}$$

$$\left(\left[E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x}) \right]_{,i} e^{-\iota \kappa_k x_k} - \iota \kappa_i E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x})e^{-\iota \kappa_k x_k} \right)$$

$$-\iota \left(\left[E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x}) \right]_{,i} e^{-\iota \kappa_k x_k} - \iota \kappa_i E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k} \right) = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x})e^{-\iota \kappa_k x_k}$$

$$\left(\left[E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x}) \right]_{,i} - \iota \kappa_i E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x}) \right)$$

$$-\iota \left(\left[E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x}) \right]_{,i} - \iota \kappa_i E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x}) \right) = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x}) \tag{4}$$

5.1.2 Transformed strong forms

General case

$$\left(\left[E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x}) \right]_{,i} - \kappa_i E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x}) \right) - \iota \left(\left[E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x}) \right]_{,i} + \kappa_i E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x}) \right) = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x}) \tag{5}$$

Isotropic modulus i.e. $E_{ij}(\boldsymbol{x}) = E(\boldsymbol{x})\delta_{ij}$:

$$\left(\left[E(\boldsymbol{x})\tilde{u}_{,i}(\boldsymbol{x}) \right]_{,i} - \kappa_i E(\boldsymbol{x})\kappa_i \tilde{u}(\boldsymbol{x}) \right) - \iota \left(\left[E(\boldsymbol{x})\kappa_i \tilde{u}(\boldsymbol{x}) \right]_{,i} + \kappa_i E(\boldsymbol{x})\tilde{u}_{,i}(\boldsymbol{x}) \right) = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x}) \tag{6}$$

Piecewise constant modulus i.e. $E_{ij,k}(\boldsymbol{x}) = 0$:

$$\left(E_{ij}(\boldsymbol{x})\tilde{u}_{,ji}(\boldsymbol{x}) - \kappa_i E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}(\boldsymbol{x}) \right) - \iota \left(E_{ij}(\boldsymbol{x})\kappa_j \tilde{u}_{,i}(\boldsymbol{x}) + \kappa_i E_{ij}(\boldsymbol{x})\tilde{u}_{,j}(\boldsymbol{x}) \right) = -\omega^2 \rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x}) \tag{7}$$

Piecewise constant isotropic modulus

$$E(\boldsymbol{x})\Big(\tilde{u}_{,ii}(\boldsymbol{x}) - \kappa_i\kappa_i\tilde{u}(\boldsymbol{x})\Big) - \iota E(\boldsymbol{x})\Big(\kappa_i\tilde{u}_{,i}(\boldsymbol{x}) + \kappa_i\tilde{u}_{,i}(\boldsymbol{x})\Big) = -\omega^2\rho(\boldsymbol{x})\tilde{u}(\boldsymbol{x}) \tag{8}$$

5.1.3 Derivation of weak forms

The weak form is obtained by multiplying the strong form (5) with the complex conjugate $\bar{v}$ of a test function v and integrating over the unit cell. The test function is periodic on the unit cell. We derive the weak form for the general case first, then specialize it to the other three cases (6-8). For conciseness, we omit the function notation "$(\boldsymbol{x})$", but it is to be understood that the trial and test functions $\tilde{u}$ and v, as well as the modulus E_{ij} and density ρ, are functions of position.

General case

$$\int_\Omega \Big([E_{ij}\tilde{u}_{,j}]_{,i} - \kappa_i E_{ij}\kappa_j\tilde{u}\Big)\bar{v}\,\mathrm{d}x - \iota\int_\Omega \Big([E_{ij}\kappa_j\tilde{u}]_{,i} + \kappa_i E_{ij}\tilde{u}_{,j}\Big)\bar{v}\,\mathrm{d}x = -\omega^2\int_\Omega \rho\tilde{u}\bar{v}\,\mathrm{d}x$$

$$\int_\Omega [E_{ij}\tilde{u}_{,j}]_{,i}\,\bar{v}\,\mathrm{d}x - \int_\Omega \kappa_i E_{ij}\kappa_j\tilde{u}\bar{v}\,\mathrm{d}x - \iota\int_\Omega [E_{ij}\kappa_j\tilde{u}]_{,i}\,\bar{v}\,\mathrm{d}x - \iota\int_\Omega \kappa_i E_{ij}\tilde{u}_{,j}\bar{v}\,\mathrm{d}x = -\omega^2\int_\Omega \rho\tilde{u}\bar{v}\,\mathrm{d}x$$

$$\int_\Omega \Big([E_{ij}\tilde{u}_{,j}\bar{v}]_{,i} - E_{ij}\tilde{u}_{,j}\bar{v}_{,i}\Big)\,\mathrm{d}x - \int_\Omega \kappa_i E_{ij}\kappa_j\tilde{u}\bar{v}\,\mathrm{d}x$$

$$-\iota\int_\Omega \Big([E_{ij}\kappa_j\tilde{u}\bar{v}]_{,i} - E_{ij}\kappa_j\tilde{u}\bar{v}_{,i}\Big)\,\mathrm{d}x - \iota\int_\Omega \kappa_i E_{ij}\tilde{u}_{,j}\bar{v}\,\mathrm{d}x = -\omega^2\int_\Omega \rho\tilde{u}\bar{v}\,\mathrm{d}x$$

$$\int_{\partial\Omega} E_{ij}\tilde{u}_{,j}\bar{v}n_i\,\mathrm{d}s - \int_\Omega E_{ij}\tilde{u}_{,j}\bar{v}_{,i}\,\mathrm{d}x - \int_\Omega \kappa_i E_{ij}\kappa_j\tilde{u}\bar{v}\,\mathrm{d}x$$

$$-\iota\int_{\partial\Omega} E_{ij}\kappa_j\tilde{u}\bar{v}n_i\,\mathrm{d}s + \iota\int_\Omega E_{ij}\kappa_j\tilde{u}\bar{v}_{,i}\,\mathrm{d}x - \iota\int_\Omega \kappa_i E_{ij}\tilde{u}_{,j}\bar{v}\,\mathrm{d}x = -\omega^2\int_\Omega \rho\tilde{u}\bar{v}\,\mathrm{d}x$$

The surface integrals are identically 0 because of the periodicity of $\tilde{u}$ and v and can be dropped, leading to the transformed weak for for the general case:

$$-\int_\Omega E_{ij}\tilde{u}_{,j}\bar{v}_{,i}\,\mathrm{d}x - \int_\Omega \kappa_i E_{ij}\kappa_j\tilde{u}\bar{v}\,\mathrm{d}x + \iota\int_\Omega E_{ij}\kappa_j\tilde{u}\bar{v}_{,i}\,\mathrm{d}x - \iota\int_\Omega \kappa_i E_{ij}\tilde{u}_{,j}\bar{v}\,\mathrm{d}x = -\omega^2\int_\Omega \rho\tilde{u}\bar{v}\,\mathrm{d}x$$

5.1.4 Transformed weak forms

General case

$$-\int_\Omega E_{ij}\tilde{u}_{,j}\bar{v}_{,i}\,\mathrm{d}x - \int_\Omega \kappa_i E_{ij}\kappa_j\tilde{u}\bar{v}\,\mathrm{d}x + \iota\int_\Omega \left(\tilde{u}\bar{v}_{,i}E_{ij}\kappa_j - \kappa_i E_{ij}\tilde{u}_{,j}\bar{v}\right)\,\mathrm{d}x = -\omega^2\int_\Omega \rho\tilde{u}\bar{v}\,\mathrm{d}x \tag{9}$$

When $\boldsymbol{E}$ is real and symmetric, (9) is Hermitian and the eigenvalues are real, as expected.

Isotropic modulus   i.e. $E_{ij}(\boldsymbol{x}) = E(\boldsymbol{x})\delta_{ij}$

$$-\int_\Omega E\tilde{u}_{,i}\bar{v}_{,i}\,\mathrm{d}x - \int_\Omega \kappa_i E\kappa_i\tilde{u}\bar{v}\,\mathrm{d}x + \iota\int_\Omega E\kappa_i\left(\tilde{u}\bar{v}_{,i} - \tilde{u}_{,i}\bar{v}\right)\,\mathrm{d}x = -\omega^2\int_\Omega \rho\tilde{u}\bar{v}\,\mathrm{d}x \tag{10}$$

4

Piecewise constant modulus Because the weak form (9) does not involve derivatives of the modulus, the weak forms for piecewise constant modulus and piecewise constant isotropic modulus are the same as (9-10), respectively.

5.2   Elasticity equation