Linearizing the photonic band structure eigenvalue problem using the Dirichlet-to-Neumann map

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Abstract

I try to make mathematical sense and extract the key idea of J. Yuan *et al.* , J. Comput. Phys. **227** (2008), which enables a linear eigenvalue problem to be expressed in one of the Bloch phases. This is potentially a much more promising way to compute the photonic band structure than the traditional (nonlinear) eigenvalue problem in the frequency parameter.

1 Set-up and definitions

The 2D unit cell T with boundary $\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$ is shown in Fig. 1. The lattice vectors are $\mathbf{e}_1$ and $\mathbf{e}_2$, and the unit surface normals $\mathbf{n}$ have signs as shown. There is some interior material region Ω; for simplicity let's take the case of a metal with Dirichlet BCs, although none of the below depends on the interior problem, as long as it is linear in the field (it need not be so in ω), and Ω does not intersect Γ. A Bloch wave (eigenfunction) is a nontrivial solution $u(\mathbf{x})$ for $\mathbf{x} \in T$ of

$$\begin{aligned} (\Delta + \omega)u &= 0 \qquad \text{in } T \setminus \Omega, &(1)\\ u &= 0 \qquad \text{on } \partial\Omega, &(2)\end{aligned}$$

which satisfies the quasi-periodicity conditions

$$\left.\begin{aligned} u(\mathbf{x}+\mathbf{e}_1) &= \alpha u(\mathbf{x}) \\ u_n(\mathbf{x}+\mathbf{e}_1) &= \alpha u_n(\mathbf{x}) \end{aligned}\right\} \quad \mathbf{x} \in \Gamma_2 \qquad \text{(QPv)}, \tag{3}$$

and

$$\left.\begin{aligned} u(\mathbf{x}+\mathbf{e}_2) &= \beta u(\mathbf{x}) \\ u_n(\mathbf{x}+\mathbf{e}_2) &= \beta u_n(\mathbf{x}) \end{aligned}\right\} \quad \mathbf{x} \in \Gamma_1 \qquad \text{(QPu)}. \tag{4}$$

The phases $\alpha, \beta \in \mathbb{C}$ lie on the unit circle: $\alpha = e^{i\mathbf{k}\cdot\mathbf{e}_1}$ and $\beta = e^{i\mathbf{k}\cdot\mathbf{e}_2}$ where $\mathbf{k}$ is the Bloch wavevector. By tiling the plane we see that the above is equivalent to finding a nontrivial solution to a periodic material problem in $\mathbf{x} \in \mathbb{R}^2$ having

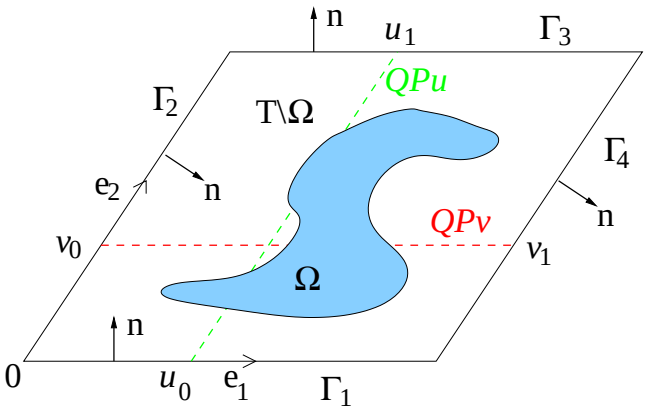

Figure 1: Geometry for 2D photonic bands problem. Dotted lines illustrate the quasiperiodicity conditions QPu (vertical) and QPv (horizontal)

the Bloch form $u(\mathbf{x}) = U(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}$ where U is periodic. Nontrivial solutions exist only for (ω, α, β) triples lying on 2D sheets (the band structure) embedded in $(0,\infty) \times S^1 \times S^1$. Traditionally the "frequency" ω is the eigenvalue and α, β are fixed parameters. In contrast, below ω, β will be fixed parameters, and α becomes the eigenvalue. (In [1] α, β are known as ρ_1, ρ_2, and we will derive their Eq. (29), although in better ways).

The interior problem (1), (2) with given Dirichlet data on Γ has a unique solution unless ω is a resonance of the "single unit cell problem", in this case a Dirichlet eigenmode of the non-simply connected domain $T \setminus \Omega$. Note that these discrete ω values depend on Ω but not α, β, and are apparently unrelated to the band structure. Thus for ω not such a value, the interior DtN map $\Lambda(\omega)$ of the unit cell is well defined by

$$u_n|_\Gamma = \Lambda u|_\Gamma, \qquad \forall u \in C(\Gamma). \tag{5}$$

It has the character of a differentiation operator, *i.e.* if the domain T were smooth it would be bounded $L^2(\Gamma) \to H^{-1}(\Gamma)$. (In fact T has corners—need to find the relevant space). Note that this differs from the *exterior* free space radiative DtN map which is commonly used to apply radiation BCs.

2 Reducing the DtN using QPu

Λ is the full DtN operator which we may write in block structure based on the four boundary lines (see Fig. 1), following similar notation to [1],

$$\begin{bmatrix} u_{0n} \\ v_{0n} \\ u_{1n} \\ v_{1n} \end{bmatrix} = \begin{bmatrix} \Lambda_{11} & \Lambda_{12} & \Lambda_{13} & \Lambda_{14} \\ \Lambda_{21} & \Lambda_{22} & \Lambda_{23} & \Lambda_{24} \\ \Lambda_{31} & \Lambda_{32} & \Lambda_{33} & \Lambda_{34} \\ \Lambda_{41} & \Lambda_{42} & \Lambda_{43} & \Lambda_{44} \end{bmatrix} \begin{bmatrix} u_0 \\ v_0 \\ u_1 \\ v_1 \end{bmatrix} \tag{6}$$

I prefer to reorder this (13)(24) into 2x2 blocks (*i.e.* u's then v's) giving

$$\begin{bmatrix} u_n \\ v_n \end{bmatrix} = \begin{bmatrix} \Lambda_{uu} & \Lambda_{uv} \\ \Lambda_{vu} & \Lambda_{vv} \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \tag{7}$$

where $u = \begin{bmatrix} u_0 \\ u_1 \end{bmatrix}$, etc, and $\Lambda_{uu} = \begin{bmatrix} \Lambda_{11} & \Lambda_{13} \\ \Lambda_{31} & \Lambda_{33} \end{bmatrix}$, etc. Using the 1st and 3rd rows of (6) to write out $u_{1n} = \beta u_{0n}$, we get after eliminating u_1 using $u_1 = \beta u_0$,

$$(\Lambda_{31} + \beta\Lambda_{33})u_0 + \Lambda_{32}v_0 + \Lambda_{34}v_1 \;=\; \beta(\Lambda_{11} + \beta\Lambda_{13})u_0 + \beta\Lambda_{12}v_0 + \beta\Lambda_{14}v_1 \tag{8}$$

Gathering terms we get

$$Du_0 := \begin{bmatrix} -\beta & 1 \end{bmatrix} \Lambda_{uu} \begin{bmatrix} 1 \\ \beta \end{bmatrix} u_0 \;=\; -\begin{bmatrix} -\beta & 1 \end{bmatrix} \Lambda_{uv} \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} \tag{9}$$

Here D can be interpreted as the operator which maps u_0 to the QPu derivative discrepancy $-\beta u_{0n} + u_{1n}$, in the Dirichlet BVP where the other walls have values $u_1 = \beta u_0$ and $v_0 = v_1 = 0$. (Note D has opposite sign to [1], and involves u rather than v). For certain (ω, β) values (curves of a 1D band structure in $(0,\infty) \times S^1$) the equation $Du_0 = 0$ will have nontrivial solutions, so D^{-1} will not exist. (9) means top and bottom values (u's) are uniquely given in terms of left and right values (v's) iff D^{-1} exists. Substituting the solution u_0 (then $u_1 = \beta u_0$) in terms of v values into (6) gives a reduced DtN map,

$$\begin{bmatrix} v_{0n} \\ v_{1n} \end{bmatrix} = M \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} = \begin{bmatrix} M_{22} & M_{24} \\ M_{42} & M_{44} \end{bmatrix} \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} \tag{10}$$

(note my notation differs from that in (28) of [1]) where the reduced DtN operator M relates only v's and has 2x2 block form

$$M = \Lambda_{vv} - \Lambda_{vu} \begin{bmatrix} 1 \\ \beta \end{bmatrix} D^{-1} \begin{bmatrix} -\beta & 1 \end{bmatrix} \Lambda_{uv} \tag{11}$$

Note that M is independent of α. This is in the form of an (operator) Schur complement of the entry Λ_{uu} in (7). We now make this statement precise.

2.1 Schur complement version of DtN reduction

The above can be derived more transparently starting from (7). Assume only the value (not derivative) parts of QPu and QPv are enforced, that is $u_1 = \beta u_0$ and $v_1 = \alpha v_0$. Derivative *error* functions $\tilde{u}_n := -\beta u_{0n} + u_{1n}$ and $\tilde{v}_n := -\beta v_{0n} + v_{1n}$ are then given using a 2x2 block operator,

$$\begin{bmatrix} D_{uu} & D_{uv} \\ D_{vu} & D_{vv} \end{bmatrix} \begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = \begin{bmatrix} \tilde{u}_n \\ \tilde{v}_n \end{bmatrix} , \tag{12}$$

where for $i,j = u,v$ we define $D_{ij} = \begin{bmatrix} -\gamma_i & 1 \end{bmatrix} \Lambda_{ij} \begin{bmatrix} 1 \\ \gamma_j \end{bmatrix}$, where $\gamma_u = \beta$ and $\gamma_v = \alpha$. Note $D_{uu} = D$ as defined in (9). The key is that D_{uu} is invertible iff (ω, β) does not lie on some 1D band structure (discussed above) for the homogeneous ($v_0 = v_1 = 0$) "horizontal cylinder" problem with the full QPu enforced. The name "cylinder" is appropriate since QPu glues top to bottom of T. Viewing (12) as a linear system for $\begin{bmatrix} u_0 \\ v_0 \end{bmatrix}$, we may apply the usual Schur complement formula, setting $\tilde{u}_n = 0$ (from QPu), namely

$$\tilde{v}_n = \tilde{D}_{vv} v_0 := \left(D_{vv} - D_{vu} D_{uu}^{-1} D_{uv} \right) v_0 \ . \tag{13}$$

This is equivalent to computing the derivative errors with (11). Note that

$$\tilde{D}_{vv} = \begin{bmatrix} -\alpha & 1 \end{bmatrix} M \begin{bmatrix} 1 \\ \alpha \end{bmatrix} \tag{14}$$

depends quadratically on α.

3 The linear eigenvalue problem in QPv

In the previous section we used both parts of QPu to compute a reduced DtN map (10) whose operator entries involved those of the full DtN map. This reduced map solves the horizontal cylinder Dirichlet BVP where only v values are given, spitting out the derivatives v_n. We simplified further (by applying just the value part of QPv) to (13) which gives the v_n derivative error function in terms of v_0.

There exists a Bloch eigenfunction of the 2D problem if $\tilde{D}_{vv}$ has a nontrivial nullspace. (Is this iff? Consider case of $v_0 = \tilde{v}_n = 0$?) This is a quadratic eigenvalue problem in α. However, as is standard for such problems we can make this linear at the cost of becoming twice the size. One such way is equivalent to going back to (10) and making the eigenfunction $\begin{bmatrix} v_0 \\ v_1 \end{bmatrix}$. The two equations enforcing the value and derivative parts of QPv restectively are

$$\begin{bmatrix} -\alpha & 1 \end{bmatrix} M \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad \begin{bmatrix} -\alpha & 1 \end{bmatrix} \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{15}$$

Stacking these as a matrix gives an operator linear generalized eigenproblem

$$\begin{bmatrix} M_{42} & M_{44} \\ 0 & I \end{bmatrix} \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} = \alpha \begin{bmatrix} M_{22} & M_{24} \\ I & 0 \end{bmatrix} \begin{bmatrix} v_0 \\ v_1 \end{bmatrix}. \tag{16}$$

The form used in [1] is different, and also follows from (14). The equation pair

$$\begin{bmatrix} M_{22} & M_{24} \end{bmatrix} \begin{bmatrix} 1 \\ \alpha \end{bmatrix} v_0 = w, \qquad \begin{bmatrix} M_{42} & M_{44} \end{bmatrix} \begin{bmatrix} 1 \\ \alpha \end{bmatrix} v_0 = \alpha w, \tag{17}$$

are equivalent to (14). They are two homogenous linear equations in v_0 and w $(= v_{0n})$, which when stacked as a 2x2 block, and separated by α give

$$\begin{bmatrix} M_{22} & -I \\ M_{42} & 0 \end{bmatrix} \begin{bmatrix} v_0 \\ v_{0n} \end{bmatrix} = \alpha \begin{bmatrix} -M_{24} & 0 \\ -M_{44} & I \end{bmatrix} \begin{bmatrix} v_0 \\ v_{0n} \end{bmatrix}. \tag{18}$$

This is (29) in [1]. I've no idea which of the above linearizations is better.

In their method, all operators are approximated by matrices in an ad-hoc way that I haven't thought much about yet.

4 Discussion

- Applying QPu first is equivalent to performing the line sum in the $\mathbf{e}_2$ direction only, for the lattice sum formulation. No obvious linearization of lattice sums yet, have to start looking.
- The interior resonant ω values at which the DtN map has a pole differ from the values $\omega = |\mathbf{k} + n\mathbf{b}_1 + m\mathbf{b}_2|^2$, $n, m \in \mathbb{Z}$, at which all lattice sum constants diverge to infinity. Here $\mathbf{b}_1$, $\mathbf{b}_2$ are the reciprocal lattice vectors complementary to $\mathbf{e}_1$, $\mathbf{e}_2$. This suggests a fundamental difference between the two mechanisms. However, both have to contend with places in the band structure where the methods break down.
- The emphasis on Dirichlet BVP seems non-essential. If reformulated using Robin BCs I believe the troublesome resonant ω values and (ω, β) pairs move, allowing access to the inaccessible band structure. This hopefully invalidates my previous point. Have to work out.
- It feels like the quadratic rather than linear eigenvalue problem is the more fundamental object in this method.

References

[1] J. Yuan, Y. Y. Lu, and X. Antoine. Modeling photonic crystals by boundary integral equations and Dirichlet-to-Neumann maps. *J. Comput. Phys.*, 227:4617–4629, 2008.