Accurate and Robust Computation of Photonic Crystal Band Structure using Second-Kind Integral Equations

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Abstract

Computing the band structure of photonic crystals is an important and numerically challenging PDE eigenvalue problem dependent on parameters (the Bloch phases). We introduce a new approach: imposing the boundary conditions on the unit-cell walls using layer potentials, and a finite number of images, resulting in a second-kind integral equation with smooth data. Unlike standard methods, which construct the quasi-periodic Greens function, our method does not break down at the (spurious) resonances of the empty torus. It couples to existing boundary-integral methods (including high-order quadratures and Fast Multipole acceleration) in a natural way. It enables piecewise-constant dielectric functions to be analyzed quickly with spectral accuracy, unlike commonly-used finite-difference and plane-wave methods.

Introduction

Periodic piecewise-constant dielectric structures are finding a rapidly growing range of exciting applications to integrated optical devices, sensors, bandgap and negative-index materials. Their most important property is their band structure; solving this is computationally intensive, yet is essential to the design and optimization of practical devices.

We consider a z-invariant structure with TM polarization; this is a doubly-periodic problem in 2D. The unit cell U has general lattice vectors $\mathbf{e}_1, \mathbf{e}_2 \in \mathbb{R}^2$ (Fig. 1) and contains a (disconnected) smooth inclusion Ω of refractive index n, $U \setminus \Omega$ having index 1. We seek Bloch waves (of time-dependence $e^{-i\omega t}$) of the form $u(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\tilde{u}(\mathbf{x})$ where $\tilde{u}$ is periodic and $\mathbf{k} = (k_x, k_y)$ is the (real-valued) Bloch wavevector. This is a PDE eigenvalue problem on a torus,

$$(\Delta + \omega^2)u = 0 \qquad \text{in } U \setminus \Omega, \tag{1}$$
$$(\Delta + n^2\omega^2)u = 0 \qquad \text{in } \Omega, \tag{2}$$

with continuity conditions on the inclusion (u_n is the normal derivative, u^+ and u^- the usual outside and inside limits on $\partial\Omega$),

$$h := u^+ - u^- = 0, \quad h' := {u_n}^+ - {u_n}^- = 0, \tag{3}$$

and quasi-periodicity conditions pairing the left-right and bottom-top walls (Fig. 1),

$$f := u|_L - \alpha^{-1}u|_{L+\mathbf{e}_1} = 0 \tag{4}$$
$$f' := u_n|_L - \alpha^{-1}u_n|_{L+\mathbf{e}_1} = 0 \tag{5}$$
$$g := u|_B - \beta^{-1}u|_{B+\mathbf{e}_2} = 0 \tag{6}$$
$$g' := u_n|_B - \beta^{-1}u_n|_{B+\mathbf{e}_2} = 0 \tag{7}$$

where $\alpha := e^{i\mathbf{k}\cdot\mathbf{e}_1}$ and $\beta := e^{i\mathbf{k}\cdot\mathbf{e}_2}$ are Bloch phases. The band structure is the subset of the parameter space (ω, α, β) for which nontrivial solutions u exist.

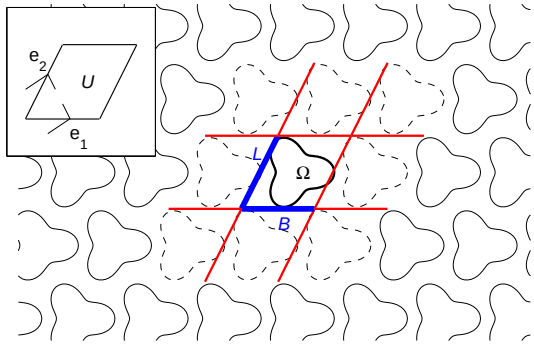

Figure 1: Unit cell U (inset), inclusion Ω, dielectric crystal lattice, and quasi-periodizing layer potentials (L, B, and red "tic-tac-toe" board).

Existing approaches include: i) low-order finite-difference and plane-wave methods [1], ii) integral equations on $\partial\Omega$ using a quasi-periodized kernel (*e.g.* [2]) $G_{\rm QP}(\mathbf{x}) := \sum_{m,n\in\mathbb{Z}} G(\mathbf{x} + m\mathbf{e}_1 + n\mathbf{e}_2)$, often evaluated via lattice sums, where $G(\mathbf{x})$ is the fundamental solution to (1). A problem not widely appreciated is that $G_{\rm QP}$ diverges (has poles) at eigenvalues of the 'empty torus' (the problem *without* inclusions), and this causes breakdown of method ii) at these spurious eigenvalues. Methods immune to this exist [3], but are ill-conditioned. Our proposal cures the problem by representing u with usual layer potentials on $\partial\Omega$ (and the 3x3 neighboring copies,

shown as dashed in Fig. 1), plus layer potentials on L and B (and 'ghost' copies in the form of a "tic-tac-toe" board). This use of carefully-phased neighboring copies causes cancellations resulting in second-kind, hence well-conditioned, integral equations.

1 Method and Results

We use standard abbreviations S (D) for the single (double) layer boundary integral operators. Inside Ω we use $u = D^{(i)}\nu + S^{(i)}\mu$, where (i) indicates interior wavenumber $n\omega$. In $U \setminus \Omega$ we use $u = \sum_{m,n\in\{-1,0,1\}} \alpha^m \beta^n (D_{mn}\nu + S_{mn}\mu) + u_{\rm QP}$, where mn indicates the density lies on inclusion copy $\partial\Omega + m\mathbf{e}_1 + n\mathbf{e}_2$. Note that the m=n=0 term plus the choice inside Ω form a familiar hypersingular-canceling representation for the transmission scattering problem [4]. $u_{\rm QP}$ accounts for the effect of the infinite sum of distant inclusion sources (solid lines in Fig. 1); we use $u_{\rm QP} = \sum_{m\in\{0,1\},n\in\{-1,0,1\}} \alpha^m \beta^n (D_{L,mn}\tau_L + S_{L,mn}\sigma_L) + \sum_{m\in\{-1,0,1\},n\in\{0,1\}} \alpha^m \beta^n (D_{B,mn}\tau_B + S_{B,mn}\sigma_B)$. Stacking density functions $\eta := [\mu;\nu]$ and $\xi = [\tau_L;\sigma_L;\tau_B;\sigma_B]$, the operator equations take the block form

$$\begin{bmatrix} A & B \\ C & Q \end{bmatrix} \begin{bmatrix} \eta \\ \xi \end{bmatrix} = \begin{bmatrix} H \\ F \end{bmatrix} \qquad (8)$$

where $H := [h;h']$ and $F := [f;f';g;g']$ are the stacked 'mismatch' functions on $\partial\Omega$ and ∂U. By construction the operator is of the form Id + compact, with all interactions distant (apart from those in B which may be made effectively so). Due to careful cancellations in Q, densities sharing a corner of U do *not* interact. The eigenvalue condition is equivalent to singularity of the block operator in (8).

Nyström discretization (with Gaussian quadrature on L and B, and periodic spectral quadratures [5] for evaluation of inclusion layer potentials on $\partial\Omega$ itself) gives rapid exponential convergence, and our condition becomes a vanishing matrix determinant. For easy systems such as Fig. 1, $N_L = 20$ points per unit-cell wall and $N_{\partial\Omega} = 40$ points on $\partial\Omega$ are sufficient for errors of 10^{-12} at $k < 10$. The total matrix size $4N_L + 2N_{\partial\Omega}$ is a little more than 10^2, so a dense SVD is cheap, enabling tens of (ω, α, β) triples to be tested per second as part of an iterative root-finder.

Exploration at constant ω (Fig. 2b) is made efficient by pre-storing coefficients of A, B, C and Q in a double power-series in (α, β). Solving a cubic polynomial eigenvalue problem in α we then can bypass the root search. By careful evaluation of B, the inclusion may even intersect the unit cell wall (Fig. 2c).

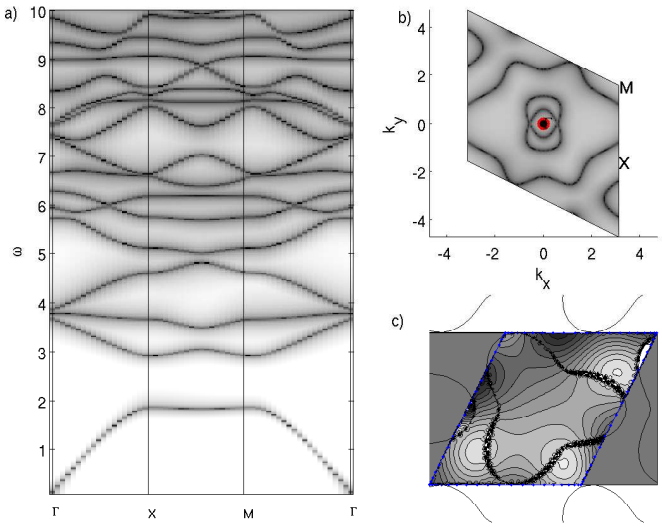

Figure 2: a) computed band structure, b) Brillouin zone slice at constant ω=7.8, and c) Bloch wave u.

Conclusions

We have solved the band structure problem efficiently with rapidly-convergent second-kind integral equations, and no quasi-periodic Green's function. Our approach generalizes to multiple inclusions, to 3D, and to grating scattering problems. It scales well to larger problems, where existing Fast Multipole scattering code can, with minor modification, replace Kress' scheme, and the dense SVD be replaced by an iterative condition number estimate.

A free, user-friendly MATLAB toolbox is in development at `http://code.google.com/p/mpspack`

References

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