Computing Floquet-Bloch modes in biperiodic slabs with Boundary Elements *†

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Abstract

A new variational formulation for the boundary element computation of Floquet-Bloch solutions to the Helmholtz equation is derived. The method is applicable to geometries that are layered in the vertical and biperiodic in two horizontal directions. The discretization leads to a nonlinear hermitian eigenvalue problem which is solved using a homotopy approach. Numerical examples demonstrate that with the boundary element approach a high accuracy can be achieved with a small number of degrees of freedom in the discretization.

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1 Introduction

Many wave propagation phenomena are characterized by nontrivial solutions to the Helmholtz equation

\[ \Delta u + k^2 n^2 u = 0, \]

in three-space. Here \( k \) is the wave number and \( n \) is a piecewise constant function that characterizes the medium of propagation.

The focus in this article is on a medium that is layered in the \( z \)-direction and has a perturbation of small \( z \)-extent that is biperiodic in the \( xy \)-plane.
The motivation comes from photonics and solid-state physics, where, for instance, photonic slab waveguides or periodic thin-film structures are of interest. Of course, many physically relevant problems are governed by the time-harmonic Schrödinger and Maxwell’s equations but we use the Helmholtz equation here as a simple model problem.

Wave propagation in periodic media is described by Floquet-Bloch theory, which is discussed extensively in the literature, see for instance [6, 7]. By now, there is a wealth of papers on computing Floquet-Bloch solutions numerically, we refer to [1, 2, 4] as representative examples. The common theme in the mentioned papers is that by using Floquet’s theorem, the problem in infinite space is reduced to a finite symmetry cell. If the PDE is discretized with finite elements or differences, the spectrum can be computed by solving a sequence of linear eigenvalue problems. Using other discretization methods it is possible to arrive at nonlinear eigenvalue problems and use path following methods [10] to compute dispersion relations quickly.

Unlike photonic crystals, photonic slabs have an infinite symmetry cell and therefore there is a continuous in addition to a discrete spectrum. Moreover, the numerical solution is more involved, as the computational domain must be truncated, and artificial boundary conditions must be imposed by a Dirichlet-to-Neumann (DtN) map. Since this map itself depends on the wave number, the resulting eigenvalue problem is always nonlinear. There are several options to handle these complications, although some are limited to the single-periodic case, see [5, 8, 13] and the survey [12]. It was shown in [14] that the boundary element method is an effective tool to solve these problems, because the size of the eigenvalue problems that have to be solved is drastically reduced. However, the approach there was based a collocation discretization, which implies that the self-adjointness of the continuous problem does not carry over to the discrete one. The primary goals of this paper are to present a new integral equation formulation in variational form and a conforming discretization which leads to a hermitian, nonlinear eigenvalue problem. We further propose a homotopy method to follow eigensolutions beginning with a planar structure.

In section 2 we give a more precise statement of the problem and provide some background material. A more detailed discussion can be found in the above mentioned literature, the goal of this section is to fix notations and make the paper self-consistent. The following section 3 derives the variational form of the boundary integral formulation and shows its equivalence with the original problem. We then discuss in section 4 suitable finite-element spaces.
for the discretization which is followed by the description of the homotopy method. Finally, section 6 presents the dispersion curves of some biperiodic structures that were obtained with an implementation of the method.

## 2 Preliminaries

**Geometry Description** We assume that \( n > 0 \) is a piecewise constant biperiodic function

\[
n(x + l_x d_x, y + l_y d_y, z) = n(x), \quad (l_x, l_y) \in \mathbb{Z}^2,
\]

where \( x = (x, y, z) \) and \( \Omega = (0, d_x) \times (0, d_y) \times \mathbb{R} \) is a fundamental periodic cell. Furthermore, we assume that \( \Omega \) can be decomposed into two semi-infinite domains \( \Omega^+ \) and \( \Omega^- \) and a finite domain \( \Omega^0 = (0, d_x) \times (0, d_y) \times (z_{-\infty}, z_{+\infty}) \) such that

\[
\bar{\Omega} = \bar{\Omega}^- \cup \bar{\Omega}^0 \cup \bar{\Omega}^+.
\]

In the semi-infinite regions \( \Omega^\pm \) the function \( n \) assumes the constant values \( n_\pm \). The domain \( \Omega^0 \) contains the biperiodic perturbation from the planar geometry, which can be decomposed into domains \( \Omega^l \) where \( n \) assumes the constant \( n_l \) such that

\[
\bar{\Omega}^0 = \bigcup_{l=1}^{L} \bar{\Omega}^l.
\]

We assume that the domains are Lipschitz with boundaries \( \Gamma_l := \partial \Omega^l \).

The interface between \( \Omega^0 \) and \( \Omega^\pm \) is denoted by \( \Gamma_z = \Gamma_x^+ \cup \Gamma_x^- \). The other boundaries of \( \Omega^0 \) are denoted by \( \Gamma_x = \Gamma_x^+ \cup \Gamma_x^- \) and \( \Gamma_y = \Gamma_y^+ \cup \Gamma_y^- \), respectively. The surface \( \Gamma \) is the union of all interfaces in \( \Omega^0 \)

\[
\Gamma = \bigcup_{l=1}^{L} \Gamma^l,
\]

and \( \Gamma_0 \) denotes all interior interfaces. A two-dimensional illustration is shown in Figure 1.

**Floquet-Bloch Solutions** We seek to compute the Floquet-Bloch solutions of the Helmholtz problem, which are nontrivial solutions of (1) of the form

\[
u(x, y, z) = \exp(i\beta_x x + i\beta_y y)\nu(x, y, z), \quad (2)
\]

where \( \beta = \beta(k) = (\beta_x, \beta_y) \in \mathbb{R}^2 \) is the unknown propagation vector and \( \nu \) is periodic in \( x \) and \( y \) with periods \( d_x \) and \( d_y \).
Figure 1: Two dimensional illustration of the geometry

An equivalent characterization is to seek $\beta$ and $k$ such that (1) in $\Omega$ with quasi periodic boundary conditions
\[
\begin{align*}
    u(0,y,z) &= e^{i\beta x} u(d_x, y, z), \\
    u(x,0,z) &= e^{i\beta y} u(x, d_y, z), \\
    \frac{\partial u}{\partial n}(0,y,z) &= -e^{i\beta d_x} \frac{\partial u}{\partial n}(d_x, y, z), \\
    \frac{\partial u}{\partial n}(x,0,z) &= -e^{i\beta d_y} \frac{\partial u}{\partial n}(x, d_y, z).
\end{align*}
\]
has nontrivial solutions. We will also use the more compact notation
\[
B_\beta^+ u = 0 \quad \text{and} \quad B_\beta^- \frac{\partial u}{\partial n} = 0
\]
(3)
to indicate that $u$ and its normal derivative satisfy quasi periodic boundary conditions.

Note that the conditions (3) are periodic in $\beta$, hence it suffices to seek solutions in the Brillouin zone
\[
\beta \in \mathbb{B} := \left[0, \frac{2\pi}{d_x}\right] \times \left[0, \frac{2\pi}{d_y}\right].
\]
(4)
DtN operator  To obtain well-posed problems it is necessary to specify radiation conditions for $|z| \to \infty$. Our primary goal is to compute modes that are guided by the structure, that is, the propagation vector $\beta$ is real and the fields decay away from the grating region. This condition will enable us to truncate the computational domain in the $z$-direction and impose an artificial boundary condition by the DtN operator. To that end, consider for a given frequency and propagation vector the Helmholtz equation with Dirichlet conditions in the semi-infinite region $\Omega^+$

$$
\begin{align*}
\Delta u + k^2 n^2 u &= 0, \quad \text{in } \Omega^+, \\
B_\beta \frac{\partial u}{\partial n} &= B_\beta^+ u = 0, \\
\quad \quad u &= f_+, \quad \text{on } \Gamma^+_z.
\end{align*}
$$

(5)

Since $n_+$ is constant, the solution can be found by separation of variables. It follows that

$$
 u(x, y, z) = \sum_{l \in \mathbb{Z}^2} f_l^+ \exp \left( i \beta_{lx} x + i \beta_{ly} y \right) \exp \left( - \alpha_l z \right)
$$

(6)

where $l = (l_x, l_y)$,

$$
\beta_{lx} = \beta_x + \frac{2\pi l_x}{d_x}, \quad \beta_{ly} = \beta_y + \frac{2\pi l_y}{d_y},
$$

$$
\hat{f}_l^+ = \frac{1}{d_x d_y} \int_0^{d_x} \int_0^{d_y} \exp \left( - i \beta_{lx} x - i \beta_{ly} y \right) f_+(x, y) \, dx \, dy
$$

and

$$
\alpha_l^+ = \left( \beta_{lx}^2 + \beta_{ly}^2 - n_+^2 k^2 \right)^{1/2}.
$$

Here the branch cut of the square root is on the negative real axis. Thus the number $\alpha_l^+$ is either positive real or positive imaginary, corresponding to exponentially decaying or outgoing $z$-dependence. From the expansion in (6) it follows that the DtN operator is given by

$$
\mathcal{T}^+ f^+(x, y) = - \sum_{l \in \mathbb{Z}^2} \alpha_l^+ f_l^+ \exp \left( i \beta_{lx} x + i \beta_{ly} y \right).
$$

Likewise, the DtN for the semi-infinite $\Omega^-$ is given by

$$
\mathcal{T}^- f^-(x, y) = - \sum_{l \in \mathbb{Z}^2} \alpha_l^- f_l^- \exp \left( i \beta_{lx} x + i \beta_{ly} y \right).
$$

5
where $\alpha_i^-$ and $f_i^-$ are defined analogously.

For the computation of guided modes only the values of $\beta$ and $k$ are of interest where all coefficients $\alpha_i^\pm$ are positive real. Thus we seek solutions only in the region

$$\mathbb{L} := \left\{ (\beta, k) : (\beta_{lx}^2 + \beta_{ly}^2)^{\frac{1}{2}} \leq k \min \{n^+, n^-\}, \beta \in \mathbb{B}, l \in \mathbb{Z}^2 \right\}. $$

In $(\beta, k)$-space this is the region below four cones centered at the corners of the Brillouin zone. The region above $\mathbb{L}$ is usually denoted as the light cone.

**Planar Structures** It is often instructive to consider a slab structure as a perturbation of a planar structure. For instance, in the example of figure 1, one obtains a planar structure if one sets $n_2 = n_3$. The modes of a planar structure can be obtained with the ansatz

$$u(x, y, z) = \exp(i\tilde{\beta}_x x + i\tilde{\beta}_y y)\varphi(z). \quad (7)$$

Substitution into (1) leads to the singular Sturm-Liouville problem

$$\varphi''(z) - \left|\tilde{\beta}\right|^2 \varphi(z) = k^2 n^2(z) \varphi(z), \quad z \in \mathbb{R}. \quad (8)$$

The spectrum of this problem is well understood, see, e.g. [12]. For any $|\tilde{\beta}|$ there is at most a finite number of $k$-values with $k^2 < \min(n_{ \pm}^2)$ with guided mode solutions. This is the discrete spectrum. Furthermore, every value of $k$ with $k^2 \geq \min(n_{ \pm}^2)$ has a radiation mode, which constitutes the continuous spectrum.

Of course, the planar structure can also be considered periodic. The function $u$ in (7) is a Floquet-Bloch mode in (2) if the propagation vectors satisfy

$$\tilde{\beta}_x = \beta_x + \frac{2\pi l_x}{d_x}, \quad \tilde{\beta}_y = \beta_y + \frac{2\pi l_y}{d_y},$$

for integer $(l_x, l_y)$. Hence the $k$-values found for any $\tilde{\beta}$ are also part of the Floquet-Bloch spectrum of $\beta$ as long as the above relationship between $\tilde{\beta}$ and $\beta$ is satisfied. The connection between the spectrum and the Floquet spectrum is illustrated in figure 2. Note that both spectra contain the same solutions to the Helmholtz equation. They are only different ways of labeling them.
3 Boundary Integral Formulation

To derive the boundary integral formulation, we begin with Green’s representation formula for a subdomain $\Omega^l$ with boundary $\Gamma^l := \partial \Omega^l$

$$u(x) = \int_{\Gamma^l} G_l(x, y) \frac{\partial u}{\partial n}(y) \, ds(y) - \int_{\Gamma^l} \frac{\partial}{\partial n_y} G_l(x, y) u(y) \, ds(y), \quad (9)$$

for $x \in \Omega^l$. For the Helmholtz equation of an interior domain, no radiation conditions have to be satisfied, therefore one can choose the Green’s function to be the real part of the free-space Green’s function. Thus we have

$$G_l(x, y) = \frac{\cos(\kappa^l |x - y|)}{4\pi |x - y|},$$

where $\kappa^l = kn^l$ is the wave number in domain $\Omega^l$.

Taking the trace and the normal trace on the boundary leads to two integral equations on $\Gamma_l$

$$\mathcal{V}_l \frac{\partial u}{\partial n} - \left( \frac{1}{2} + \mathcal{K}_l \right) u = 0, \quad (10)$$

$$\left( -\frac{1}{2} + \mathcal{K}_l' \right) \frac{\partial u}{\partial n} + \mathcal{D}_l u = 0, \quad (11)$$

where $\mathcal{V}_l, \mathcal{K}_l, \mathcal{K}_l'$ and $\mathcal{D}_l$ are the usual layer potentials

$$\mathcal{V}_l g(x) = \int_{\Gamma^l} G_l(x, y) g(y) \, ds(y),$$
\[ \mathcal{K}_t g(x) = \int_{\Gamma} \frac{\partial}{\partial n_y} G_t(x, y) g(y) \, ds(y), \]
\[ \mathcal{K}_t' g(x) = \int_{\Gamma} \frac{\partial}{\partial n_x} G_t(x, y) g(y) \, ds(y), \]
\[ \mathcal{D}_t g(x) = -\frac{\partial}{\partial n_x} \int_{\Gamma} \frac{\partial}{\partial n_y} G_t(x, y) g(y) \, ds(y). \]

Note that the normals here point into the exterior of \( \Omega \). With our choice of \( G_t \) the operator \( \mathcal{K}_t' \) is the adjoint of \( \mathcal{K}_t \).

A standard result in the theory of boundary integral operators is that the single layer and hypersingular operator satisfy a G\aa rding inequality [3]. That is, there are compact operators \( \mathcal{V}_t : H^{-\frac{1}{2}}(\Gamma_t) \rightarrow H^{-\frac{3}{2}}(\Gamma_t) \) and \( \mathcal{C}_t^d : H^{\frac{3}{2}}(\Gamma_t) \rightarrow H^{-\frac{1}{2}}(\Gamma_t) \) and positive constants \( c_v \) and \( c_d \) such that
\[
\langle \psi_t, (\mathcal{V}_t + \mathcal{C}_t^v) \psi_t \rangle \geq c_v \| \psi_t \|_{H^{-\frac{1}{2}}(\Gamma_t)}^2, \quad (12)
\]
\[
\langle \varphi_t, (\mathcal{D}_t + \mathcal{C}_t^d) \varphi_t \rangle \geq c_d \| \varphi_t \|_{H^{\frac{1}{2}}(\Gamma_t)}^2, \quad (13)
\]
for all \( \psi_t \in H^{-\frac{1}{2}}(\Gamma_t) \) and \( \varphi_t \in H^{\frac{3}{2}}(\Gamma_t) \). Here, \( \langle \cdot, \cdot \rangle \) denotes the duality pairing between \( H^{\frac{1}{2}}(\Gamma_t) \) and \( H^{-\frac{1}{2}}(\Gamma_t) \). Moreover, the operators \( \mathcal{V}_t : H^{-\frac{1}{2}}(\Gamma_t) \rightarrow H^{-\frac{3}{2}}(\Gamma_t) \), \( \mathcal{K}_t : H^{\frac{3}{2}}(\Gamma_t) \rightarrow H^{-\frac{1}{2}}(\Gamma_t) \), \( \mathcal{K}_t' : H^{-\frac{3}{2}}(\Gamma_t) \rightarrow H^{\frac{3}{2}}(\Gamma_t) \) and \( \mathcal{D}_t : H^{\frac{3}{2}}(\Gamma_t) \rightarrow H^{-\frac{3}{2}}(\Gamma_t) \) are bounded.

We define the spaces
\[ U_\beta = \left\{ (\varphi_1, \ldots, \varphi_L) : \varphi_t \in H^{\frac{3}{2}}(\Gamma_t), \varphi_t = \varphi_{t'} \text{ on } \Gamma_t \cap \Gamma_{t'} \text{ and } B_\beta^+ \varphi = 0 \right\}, \]
\[ V_\beta = \left\{ (\psi_1, \ldots, \psi_L) : \psi_t \in H^{-\frac{3}{2}}(\Gamma_t), \psi_t = -\psi_{t'} \text{ on } \Gamma_t \cap \Gamma_{t'} \text{ and } B_\beta^- \psi = 0 \right\}, \]
which are closed subspaces of \( H^{\frac{3}{2}}(\Gamma_1) \otimes \ldots \otimes H^{\frac{3}{2}}(\Gamma_L) \) and \( H^{-\frac{3}{2}}(\Gamma_1) \otimes \ldots \otimes H^{-\frac{3}{2}}(\Gamma_L) \), equipped with the norms
\[ \| \varphi \|_{H^{\frac{3}{2}}} := \left( \sum_{t=1}^L \| \varphi_t \|_{H^{\frac{3}{2}}(\Gamma_t)}^2 \right)^{\frac{1}{2}} \quad \text{and} \quad \| \psi \|_{H^{-\frac{3}{2}}} := \left( \sum_{t=1}^L \| \psi_t \|_{H^{-\frac{3}{2}}(\Gamma_t)}^2 \right)^{\frac{1}{2}}, \]
respectively.

In addition to satisfying (10) and (11) a guided mode solution is also continuous across the \( \Gamma_z \)-interfaces
\[ \frac{\partial u}{\partial n} = T^\perp u, \quad \text{on } \Gamma_z^\perp. \quad (14) \]
To derive a variational form the following observation will be useful. It follows easily because contributions of interior and periodic surfaces cancel.

**Lemma 1.** For $u, \varphi \in U_\beta$ and $v, \psi \in V_\beta$ it follows that

$$
\sum_{l=1}^L \langle \psi_l, u_l \rangle = \langle \psi, u \rangle_{\Gamma_z} \quad \text{and} \quad \sum_{l=1}^L \langle \varphi_l, v_l \rangle = \langle \varphi, v \rangle_{\Gamma_z}.
$$

To obtain a variational formulation multiply (10), (11) and (14) by test functions $\psi_l$ and $\varphi_l$, defined on the boundary $\Gamma^l$ and add all integrals. Together with lemma 1 this leads to

$$
a(\psi, \varphi; v, u) = 0,
$$

where

$$
a(\psi, \varphi; v, u) := \langle \varphi, Tu \rangle_{\Gamma_z} - \frac{1}{2} \left( \langle \psi, u \rangle_{\Gamma_z} + \langle \varphi, v \rangle_{\Gamma_z} \right)
\sum_{l=1}^L \left( \langle \psi_l, V_l v \rangle - \langle \psi_l, K_l u_l \rangle - \langle \varphi_l, K'_l v_l \rangle - \langle \varphi_l, D_l u_l \rangle \right)
$$

Evidently, the bilinear form is symmetric

$$
a(\psi, \varphi; v, u) = a(v, u; \psi, \varphi).
$$

If $u$ is a guided mode solution of (1), then $(u_1, \ldots, u_L)$ and $(v_1, \ldots, v_L)$ with $u_l = u|_{\Gamma_1}$ and $v_l := \partial u/\partial n_l$ is a solution to the variational problem: Find $(u, v) \in U_\beta \otimes V_\beta$ such that for all $(\varphi, \psi) \in V_\beta \otimes U_\beta$ (15) holds. The converse is stated in the following result.

**Theorem 2.** A nontrivial solution of (15) with $(\beta, k) \in \mathbb{L}$ extends to a guided-mode solution of (1) by

$$
\tilde{u}(x) = \begin{cases}
\int_{\Gamma_1} G_l(x, y) \frac{\partial u_l}{\partial n}(y) \, ds(y) - \int_{\Gamma^0} \frac{\partial}{\partial n_y} G_l(x, y) u_l(y) \, ds(y), & x \in \Omega^l, \\
\sum_{l \in \mathbb{Z}^2} u_l^\pm \exp \left( i \beta_l x + i \beta_y \mp \alpha_l^\pm z \right), & x \in \Omega^\pm.
\end{cases}
$$

(16)
Proof. The function defined in (16) satisfies the Helmholtz equation in every subdomain. It remains to verify that the traces and normal traces are continuous across the interfaces in the weak sense.

Let $x \in \Gamma_0$ a point on the interface between $\Omega_l$ and $\Omega_r$. The jump relations of the double layer potential implies that

$$
\tilde{u}(x^-) = \mathcal{V}_l v_l(x) - \mathcal{K}_l u_l(x) + \frac{1}{2} u_l(x),
$$

$$
\tilde{u}(x^+) = \mathcal{V}_r v_r(x) - \mathcal{K}_r u_r(x) + \frac{1}{2} u_r(x),
$$

where $x^\pm$ indicates taking the limit from the $\Omega_l$ and $\Omega_r$ side. From choosing in (15) $\varphi = 0$ and $\psi$ to be a function that is supported in a small neighborhood of $x$ one can conclude that

$$
\mathcal{V}_l v_l(x) - \mathcal{K}_l u_l(x) - \frac{1}{2} u_l(x) - \left( \mathcal{V}_r v_r(x) - \mathcal{K}_r u_r(x) - \frac{1}{2} u_r(x) \right) = 0.
$$

Mind that the minus sign comes from the fact that $\psi_l(x) = -\psi_r(x)$. From this and equations (17), (18) we can conclude that $\tilde{u}(x^-) = \tilde{u}(x^+)$. Now apply the jump relations of the normal derivative. It follows that

$$
\frac{\partial \tilde{u}}{\partial n_l}(x^-) = \mathcal{K}_l' v_l(x) + \mathcal{D}_l u_l(x) + \frac{1}{2} v_l(x),
$$

$$
\frac{\partial \tilde{u}}{\partial n_r}(x^-) = \mathcal{K}_r' v_r(x) + \mathcal{D}_r u_r(x) + \frac{1}{2} v_r(x).
$$

From choosing in (15) $\psi = 0$ and $\varphi$ to be a function that is supported in a small neighborhood of $x$ one can conclude that

$$
\mathcal{K}_l v_l(x) + \mathcal{D}_l u_l(x) - \frac{1}{2} v_l(x) + \mathcal{K}_r' v_r(x) + \mathcal{D}_r u_r(x) - \frac{1}{2} v_r(x) = 0,
$$

thus it follows from (19), (20) that

$$
\frac{\partial \tilde{u}}{\partial n_l}(x^-) = -\frac{\partial \tilde{u}}{\partial n_r}(x^+) = \frac{\partial \tilde{u}}{\partial n_r}(x^+).
$$

Now let $x \in \Gamma_z^+$ be a point on the interface of $\Omega^+$ and some interior domain, say $\Omega_l$. The jump relations (17) and (19) apply again, where $x^-$ denotes a limit as the evaluation point approaches $\Gamma_z^+$. On the other hand, from (15) we can conclude that

$$
\mathcal{V}_l v_l(x) - \mathcal{K}_l u_l(x) - \frac{1}{2} u_l(x) = 0,
$$

$$
\mathcal{K}_l' v_l(x) + \mathcal{D}_l u_l(x) - \frac{1}{2} v_l(x) + \mathcal{T} u(x) = 0.
$$
This implies that $\tilde{u}(x^-) = u_l(x)$ and that $v_l(x) = T u(x)$. Thus the trace and the normal trace are continuous across $\Gamma^+$. The continuity for $\Gamma^-$ is completely analogous.

It remains to verify the quasi continuity of $\tilde{u}$. Consider a point $x \in \Gamma_x^-$ which lies on the boundary of some subdomain, say $\Omega_l$. The periodic image $x' := x + dx e_x$ lies on the $\Gamma^+_l$ which lies on the interface of a possibly different domain $\Omega_{l'}$. By construction of $\tilde{u}$, the jump relations (17-20) hold, where $x^-$ indicates limiting value as the evaluation point approaches $x$ from $\Omega_l$ and $x^+$ a limiting value of approaching $x'$ from $\Omega_{l'}$. From the variational form we obtain

$$
\mathcal{V}_l v_l(x) - \mathcal{K}_l u_l(x) - e^{-i\beta_x dx} (\mathcal{V}_{l'} v_{l'}(x') - \mathcal{K}_{l'} u_{l'}(x')) = 0, \quad (21)
$$

$$
\mathcal{K}'_l v_l(x) + \mathcal{D}_l u_l(x) + e^{-i\beta_x dx} (\mathcal{K}'_{l'} v_{l'}(x') + \mathcal{D}_{l'} u_{l'}(x')) = 0. \quad (22)
$$

By combining (17),(18) and (21) and using $u_{l'}(x) = \exp(i\beta_x dx) u_l(x)$ it follows that

$$
\tilde{u}(x^+) - e^{-i\beta_x dx} \tilde{u}(x^-) = 0.
$$

Likewise, from (19),(20), (22) and $v_{l'}(x) = -\exp(i\beta_x dx) v_l(x)$ it follows that

$$
\frac{\partial \tilde{u}}{\partial n'}(x^+) + e^{-i\beta_x dx} \frac{\partial \tilde{u}}{\partial n}(x^-) = 0.
$$

This implies quasiperiodicity for $\Gamma_x$. The same argument for $\Gamma_y$ completes the proof.

The DtN operator induces the bilinear form

$$
\langle \varphi, T u \rangle = -\sum_{l \in \mathbb{Z}^2} (\tilde{\alpha}_l^+ \varphi_l^+ u_l^+ + \tilde{\alpha}_l^- \varphi_l^- u_l^-) \quad (23)
$$

which is bounded in $U_\beta$ and negative

$$
\langle \varphi, T \varphi \rangle \leq 0. \quad (24)
$$

The solvability of the variational form is stated in the following result.

**Theorem 3.** The nullspace of (15) is either trivial or finite dimensional.

**Proof.** To understand the solvability of (15) consider the variational formulation

$$
\tilde{a}(\psi, \varphi; v, u) := a(\psi, -\varphi; v, u) = 0. \quad (25)
$$
Clearly, (15) and (25) have the same solutions. Moreover, $\tilde{a}$ is bounded in $V_\beta \otimes U_\beta$ and

$$\tilde{a}(\psi, \varphi; \psi, \varphi) = \sum_{l=1}^{L} \left( \langle \psi, V_lv \rangle + \langle \varphi, D_lu \rangle \right) + \frac{1}{2} \left( \langle \psi, \varphi \rangle - \langle \varphi, \psi \rangle \right) - \langle \varphi, T \varphi \rangle$$

From (12) and (13) and (24) it can be concluded that there are compact operators $C_v : V_\beta \rightarrow V_\beta$ and $C_d : U_\beta \rightarrow U_\beta$ and a positive constant $c$ such that

$$\text{Re} \tilde{a}(\psi, \varphi; \psi, \varphi) + \langle \varphi, C_v \varphi \rangle + \langle \psi, C_d \psi \rangle \geq c \left( \| \varphi \|^2_{H^{\frac{1}{2}}} + \| \psi \|^2_{H^{-\frac{1}{2}}} \right)^{\frac{1}{2}}$$

Thus the bilinear form satisfies another Gårding inequality in the space $V_\beta \otimes U_\beta$. This implies the assertion.

4 Galerkin Method for the Interior Problem

To derive the Galerkin solution of (15) consider an admissible triangulation of $\Gamma$. That is, two triangles intersect either at a common edge, a common vertex or not at all. Note that it is possible that an edge is shared by more than two triangles. We also assume that the triangulation is periodic in the $x$- and $y$- directions, i.e., $\tau$ is a triangle on $\Gamma_x^+$ if and only if there is a triangle $\tau'$ on $\Gamma_x^-$ such that $\tau = \tau' + d_x e_x$ and $\tau$ is a triangle on $\Gamma_y^+$ if and only if there is a triangle $\tau'$ on $\Gamma_y^-$ such that $\tau = \tau' + d_y e_y$. The triangulation of $\Gamma$ also implies that every subdomain $\Gamma_i$ is partitioned into an admissible triangulation.

We seek the Galerkin solution in piecewise polynomial subspaces of $U_\beta$ and $V_\beta$. To that end, consider the spaces $S_{l}^{(0)}$ of piecewise constant functions subject to the triangulation of $\Gamma_i$ and $S_{l}^{(1)}$ the space of continuous and piecewise linear functions on $\Gamma_i$. Then the subspaces for the discretization are given by

$$U_{\beta}^h = \left\{ (\varphi_1, \ldots, \varphi_L) : \varphi_l \in S_{l}^{(1)}, \varphi_l = \varphi_{l'} \text{ on } \Gamma_l \cap \Gamma_{l'} \text{ and } B^{\pm}_\beta \varphi = 0 \right\},$$

$$V_{\beta}^h = \left\{ (\psi_1, \ldots, \psi_L) : \psi_l \in S_{l}^{(0)}, \psi_l = -\psi_{l'} \text{ on } \Gamma_l \cap \Gamma_{l'} \text{ and } B^{-}_\beta \psi = 0 \right\}.$$

The discretization of (15) is: Find $(v_h, u_h) \in V_{\beta}^h \otimes U_{\beta}^h$ such that for all $(\psi_h, \varphi_h) \in V_{\beta}^h \otimes U_{\beta}^h$

$$a(\psi_h, \varphi_h; v_h, u_h) = 0$$

(26)
holds. It is not hard to see that $U^h_{\beta}, V^h_{\beta}$ are subspaces of $U_{\beta}, V_{\beta}$ thus the discretization is conforming.

To obtain a basis of $U^h_{\beta}$ and $V^h_{\beta}$ consider a box functions $\chi_\tau$ for a triangle $\tau$ and a hat function $\zeta_v$ for a vertex $v$ in the triangulation of $\Gamma$. The quasiperiodic extensions of these functions are defined as

$$\chi^\beta_\tau = \begin{cases} \chi_\tau, & \text{if } \tau \subset \Gamma_0 \cup \Gamma_z, \\ \chi_\tau - e^{i\beta_x x} \chi'_{\tau}, & \text{if } \tau \subset \Gamma_x^- , \\ \chi_\tau - e^{i\beta_y y} \chi'_{\tau}, & \text{if } \tau \subset \Gamma_y^- , \end{cases}$$

and

$$\zeta^\beta_v = \begin{cases} \zeta_v, & \text{if } v \in \hat{\Gamma}_0 \cup \hat{\Gamma}_z , \\ \zeta_v + e^{i\beta_x x} \zeta'_{v}, & \text{if } v \in \Gamma_x^- \setminus \Gamma_y^- , \\ \zeta_v + e^{i\beta_y y} \zeta'_{v}, & \text{if } v \in \Gamma_y^- \setminus \Gamma_x^- , \\ \zeta_v + e^{i\beta_x x} \zeta''_{v} + e^{i\beta_y y} \zeta''_{v} + e^{i(\beta_x x + \beta_y y)} \zeta''''_{v}, & \text{if } v \in \Gamma_x^- \cap \Gamma_y^- . \end{cases}$$

Here primes denote the corresponding periodic copy of the panel or vertex. Since functions in $V^h_{\beta}$ alternate signs on interior interfaces define

$$\sigma'_{\tau} = \begin{cases} -1 & \text{if } \tau \in \bar{\Omega}_l \cap \bar{\Omega}'_{l'} \text{ and } n_l < n_{l'} , \\ 1 & \text{else} , \end{cases}$$

then the basis functions of $V^h_{\beta}$ and $U^h_{\beta}$ are

$$\chi^\beta_\tau = (\sigma^1_\tau \chi^\beta_\tau |_{\Gamma_1}, \ldots, \sigma^L_\tau \chi^\beta_\tau |_{\Gamma_L}),$$

$$\zeta^\beta_v = (\zeta^\beta_v |_{\Gamma_1}, \ldots, \zeta^\beta_v |_{\Gamma_L}).$$

With this basis the discrete variational formulation (26) can be expressed in matrix form as follows: Find $(\beta, k) \in \mathbb{L}$ such that the matrix $A_h(\beta, k)$ has a nontrivial nullspace. The matrix is given by

$$A_h(\beta, k) = \begin{bmatrix} a(\chi^\beta_\tau, \chi^\beta_{\tau'}) & a(\chi^\beta_\tau, \zeta^\beta_v) \\ a(\zeta^\beta_v, \chi^\beta_{\tau'}) & a(\zeta^\beta_v, \zeta^\beta_v) \end{bmatrix}$$

where $\tau, \tau'$ and $v, v'$ run through all triangles and vertices that appear in the above definitions of $\chi_{\beta, \tau}$ and $\zeta_{\beta, v}$. Since the bilinear form is hermitian, the matrix $A_h$ is hermitian.
Computation of the DtN operator  Some of the matrix coefficients depend on the DtN operator of (23), whose evaluation involve an infinite series. To compute this operator, we truncate the series by adding only terms in the diamond-shaped domain

\[ l \in \mathbb{Z}^2_p := \{ (l_x, l_y) \in \mathbb{Z}^2 : |l_x| + |l_y| \leq p \}. \quad (27) \]

Note that if some of the subdomains are planar it is possible to discretize only the irregularly shaped domains and incorporate the planar subdomains in the semi-infinite domains. For instance, in figure 1 one would discretize \( \Omega^2 \) and \( \Omega^3 \) and move \( \Gamma^- \) to the \( \Omega^1-\Omega^3 \)-interface and \( \Gamma^+ \) to the \( \Omega^3-\Omega^4 \)-interface. In this case the DtN operator still appears in the general form of (23), but the coefficients \( \alpha^\pm_l \) must be computed using planar layer transfer matrices. Since this process is described in the literature it is not described here. Details can be found in, e.g., [13].

5 Solution of the Eigenvalue Problem

After discretization problem (26) reduces to a nonlinear eigenvalue problem. That is, we have a matrix \( A_h \) whose coefficients depend on \( \beta \) and \( k \) and wish to find those values in \( L \) for which the matrix is singular. The conventional approach in photonics is to fix the propagation vector \( \beta \) in the Brillouin zone and to compute all values of the frequency \( k \) that lie below the light cone. However, in view of the boundary element method, it turns out that it is more efficient to fix the frequency and solve for the values of \( \beta \). The reason is that when computing \( A_h \) one first calculates the influence coefficients of the classical boundary integral operators (which depend on \( k \)) and then forms weighted combinations (which depend on \( \beta \)) to form the matrix \( A_h \). The computation of the influence coefficients is much more costly, as four-dimensional, possibly singular integrations have to be computed. If the frequency is fixed, the expensive part of the computation has to be done only once when \( \beta \) is varied.

Nonlinear Inverse Iteration  Since \( \beta \) is a vector with two components the solutions for a fixed \( k \) form curves in the Brillouin zone \( B \). We first describe how to obtain a point on such a curve beginning with an initial guess \( \beta \) and a search direction \( \nu \). Specifically, we search for the value \( t \in \mathbb{R} \) such that the matrix \( T(t) := A_h(\beta + t\nu, k) \) is singular. The latter problem is
a nonlinear eigenvalue problem for which several solution methods exist [9].
The following nonlinear version of the inverse iteration is suitable for this purpose.

choose $t^0 = 0$ and $x^0 \in \mathbb{C}^N$
for $k = 0, 1, 2\ldots$
\begin{align*}
\delta t^k &= \frac{(x^k)^H T(t^k) x^k}{(x^k)^H T'(t^k) x^k} \\
\text{solve } T(t^k) y^{k+1} &= T'(t^k) x^k \\
t^{k+1} &= t^k - \delta t^k \\
x^{k+1} &= \delta t^k x^k
\end{align*}
end

Note that in each iteration the matrix and its derivative must be re-assembled for a different propagation vector and a linear system must be solved. Since with the boundary element method the sizes of the matrices are typically very manageable, the linear solver is simply based on the $LU$-decomposition although iterative methods are feasible as well. Since $T(t^k)$ and $T'(t^k)$ are hermitian, the iterates $t^k$ are always real, whereas the vectors $x^k$ are generally complex.

To obtain the initial vector $x^0$ the conventional inverse iteration

choose $x^0$ random
for $k = 0, 1, 2\ldots$
\begin{align*}
\text{solve } T(t^0) y^{k+1} &= T'(t^0) x^k \\
x^{k+1} &= \frac{y^{k+1}}{\|y^{k+1}\|}
\end{align*}
end

$x^0 \leftarrow x^k$

is effective. Here the matrix is fixed and hence the cost of finding the initial guess is small compared to the nonlinear inverse iteration.

**Homotopy method** So far we have discussed how to find a single point on the solution curve, which, of course, depends on a good initial guess. To obtain the full curve, a path following method will not be satisfactory since solutions generally consist of several disconnected components. Therefore we employ a homotopy method based on deforming the function $n$ from a planar
waveguide, where solutions can be found easily, to the biperiodic waveguide under consideration. Specifically, we set

$$n_\lambda(x, y, z) = (1 - \lambda)n_P(z) + \lambda n(x, y, z), \quad \lambda \in [0, 1].$$  

where $n_P(z)$ is the material constant of the 'planarized' geometry that results when the value of $n$ in the irregularly shaped subdomains is replaced by their maximum.

As discussed in section 2 the dispersion curves for the planarized waveguide are four circles that are centered in the corners of the Brillouin zone. The radii are the propagation constants of the planar structure that can be found numerically, for instance, with the method of [11]. We select points on these circles which will be the initial guesses to compute the curves for the structure with parameter $0 < \lambda_1 < 1$, which in turn will serve as initial guesses for $\lambda_2 > \lambda_1$, and so on, until the final curve has been reached. The search direction $\nu$ is set to be orthogonal to the current solution curve. To determine this direction, assume that the dispersion curve is parameterized by $\theta$. If $x(\beta)$ is the eigenvector, then

$$A(\beta(\theta))x(\beta(\theta)) = 0.$$  

Differentiating with respect to $\theta$ leads to

$$\left( \frac{\partial A}{\partial \beta_x} x + A \frac{\partial x}{\partial \beta_x} \right) \frac{\partial \beta_x}{\partial \theta} + \left( \frac{\partial A}{\partial \beta_y} x + A \frac{\partial x}{\partial \beta_y} \right) \frac{\partial \beta_y}{\partial \theta} = 0.$$  

The latter two equations imply that

$$x^H \frac{\partial A}{\partial \beta_x} x \frac{\partial \beta_x}{\partial \theta} + x^H \frac{\partial A}{\partial \beta_y} x \frac{\partial \beta_y}{\partial \theta} = 0,$$

hence we see that the vector

$$\nu = \left[ \begin{array}{c} x^H \frac{\partial A}{\partial \beta_x} x \\ x^H \frac{\partial A}{\partial \beta_y} x \end{array} \right] \in \mathbb{R}^2$$

is orthogonal to the curve.
6 Numerical Results

We have tested the method on several geometries that result from perturbing a four layer planar geometry given by

\[
n_P(z) = \begin{cases} 
\sqrt{2.3}, & z < -0.5, \\
n_1, & -0.5 < z < 0, \\
n_2, & 0 < z < 0.5, \\
1, & 0.5 < z.
\end{cases}
\]

In the grating region \( z \in [0, 0.5] \) the function is replaced either by a rectangular

\[
n(x, y, z) = \begin{cases} 
1, & \text{if } (x, y) \in [0, 0.5]^2, \\
n_2, & \text{else},
\end{cases}
\]

or by a triangular perturbation

\[
n(x, y, z) = \begin{cases} 
1, & \text{if } 0 \leq x, y, x + y \leq 1, \\
n_2, & \text{else}.
\end{cases}
\]

The grating period is \( d_x = d_y = 1 \). For the values \( n_1 = n_2 = 2 \) the planar structure has one guided mode below the light cone, and for \( n_1 = n_2 = 5 \) there are two guided modes.

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Table 1: Convergence of \( \beta_x \) of the cubical perturbation.

Tables 1 and 2 display the computed values of \( \beta_x = \beta_y \) for the one-mode structure when \( k = 1.5 \) for different uniform mesh refinements and different
Table 2: Convergence of $\beta_x$ for the triangular perturbation.

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expansion orders in (27). The data makes clear that the convergence is rapid and that even with a very coarse mesh a good approximation of the actual solution can be obtained.

Figures 3 and 4 display the dispersion curves for the planar structure in lighter shade and the curves for the cubically perturbed structure in black. The regions that are not in $\mathbb{L}$ are marked in gray. The computation was done with the second refinement with 642 degrees of freedom. The homotopy method used six steps and followed 1600 points. The overall cpu time to generate one of the figures is about two to three hours. For the coarser mesh with 154 dof the cpu time is in the range of minutes and the figures would be indistinguishable at the shown resolution. Finally, figure 5 shows the evolution of the dispersion curves under the homotopy method. For clarity, we only display only every second step.

References


Figure 3: Dispersion curves for the one-mode structure
Figure 4: Dispersion curves for the two-mode structure

Figure 5: Evolution of the dispersion curve under the homotopy method. One-mode structure, $k = 1.9$. 

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