

# Dirichlet-to-Neumann transparent boundary conditions for photonic crystal wave-guides

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In this work we present a complete algorithm for the exact computation of the guided mode band structure in photonic crystal (PhC) wave-guides. In contrast to the supercell method, the used approach does not introduce any modelling error and is hence independent of the confinement of the modes. The approach is based on Dirichlet-to-Neumann (DtN) transparent boundary conditions that yield a nonlinear eigenvalue problem. For the solution of this nonlinear eigenvalue problem we present a direct technique using Chebyshev interpolation that requires a band gap calculation of the PhC in advance. For this band gap calculation — we introduce as a very efficient tool — a Taylor expansion of the PhC band structure. We show that our algorithm — like the supercell method — converges exponentially, however, its computational costs — in comparison to the supercell method — only increase moderately since the size of the matrix to be inverted remains constant.

*Index Terms*—Photonic crystals, Boundary conditions, Eigenvalues and eigenfunctions, Finite element methods, Nonlinear equations.

## I. INTRODUCTION

We consider the problem of finding guided modes in 2D PhC wave-guides. For simplicity we restrict our presentation to the transverse magnetic (TM) mode, but the whole method can directly be transferred to the transverse electric (TE) mode.

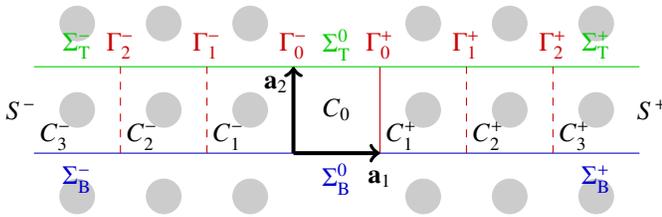


Figure 1. Sketch of the PhC wave-guide and the periodicity strip  $S = S^+ \cup C_0 \cup S^-$ , its unit cells  $C_n^\pm$  with left/right boundaries  $\Gamma_n^\pm$ , its top/bottom boundaries  $\Sigma_{T/B} = \Sigma_{T/B}^+ \cup \Sigma_{T/B}^0 \cup \Sigma_{T/B}^-$ , and its periodicity vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ .

According to the Floquet-Bloch theory [1] guided modes, which are modes that decay for  $|x_1| \rightarrow \infty$ , are represented by Bloch modes  $e_k$  that satisfy

$$-\Delta e_k - \omega^2 \varepsilon e_k = 0 \quad (1a)$$

in the infinite strip  $S = S^+ \cup C_0 \cup S^- \subset \mathbb{R}^2$ , *c.f.* Fig. 1, with quasi-periodic boundary conditions

$$e_k|_{\Sigma_T} = e^{ik|a_2|} e_k|_{\Sigma_B}, \quad \partial_n e_k|_{\Sigma_T} = -e^{ik|a_2|} \partial_n e_k|_{\Sigma_B}, \quad (1b)$$

where the parameter  $k \in B$  is the so-called quasi-momentum in the one-dimensional Brillouin zone  $B = [-\pi/|a_2|, \pi/|a_2|]$ , and the operator  $\partial_n$  denotes the normal derivative  $\partial_n = \mathbf{n} \cdot \nabla$  with the unit normal vector  $\mathbf{n}$  outward to the domain  $S$ . We assume the material to be lossless, *i. e.*, the permittivity  $\varepsilon$  is supposed to be real and positive. With the substitution  $e_k(\mathbf{x}) = e^{ikx_2} u(\mathbf{x})$ , the

eigenvalue problem (1) is equivalent to: find couples  $(\omega^2, k) \in \mathbb{R}^+ \times B$  such that there exists a guided mode  $u$  that satisfies

$$-(\nabla + ik\mathbf{a}_2) \cdot (\nabla + ik\mathbf{a}_2)u - \omega^2 \varepsilon u = 0 \quad \text{in } S \quad (2)$$

with periodic boundary conditions at the top and bottom boundaries  $\Sigma_T$  and  $\Sigma_B$ .

The frequently used supercell method [2], [3] provides access to approximations of guided modes of the eigenvalue problem (2). Based on the observation that guided modes decay exponentially with  $|x_1| \rightarrow \infty$ , the eigenvalue problem (2) is posed in a bounded supercell  $S_{sc} \subset S$  instead of the infinite strip  $S$ . This supercell  $S_{sc}$  is obtained by simply truncating the infinite strip  $S$  after  $n \in \mathbb{N}$  periodicity cells of the left and right half strips, and prescribing periodic boundary conditions at the left and right boundaries  $\Gamma_n^\pm$ . The supercell method provides access to an approximation to the solutions of (2) while introducing a modelling error that converges exponentially with the number  $n$  of periodicity cells [2], where the computational effort increases with  $n$ . In addition to this modelling error a discretization error is introduced by the numerical scheme.

In this article, we propose an effective algorithm to compute the guided mode band structure, for which only the channel cell  $C_0$  and the unit cell  $C_1$  have to be discretized. For this we use the discrete version [4] of DtN operators [5] (see Section II), which, used in a finite element discretization, leads to a non-linear matrix eigenvalue problem (see Section III). We use a Chebyshev interpolation [6], [4] using  $k$ -dependent frequency intervals to get linear matrix eigenvalue problems (see Section III). To obtain valid frequency intervals we compute  $k$ -dependent band gaps. For the efficient computation of these band gaps we introduce in Section V a new algorithm based on a Taylor expansion and derivatives of higher order. The suggested algorithm introduces no modelling error, but an interpolation error, whose convergence is studied in Section VI and compared to the modelling error of the supercell method.

Our algorithm can be extended straightforward to three-dimensional unit-cells, which are bounded, but may have a permittivity variation in  $x_3$ .

## II. NONLINEAR EIGENVALUE PROBLEM USING DtN OPERATORS

### A. Definition of the DtN operators

Let us introduce Dirichlet problems in the infinite half-strips  $S^\pm$ : for any Dirichlet data  $\varphi$  on  $\Gamma_0^\pm$  find  $u^\pm(\varphi) \equiv u^\pm(\cdot; \omega, k, \varphi)$  such that

$$-(\nabla + i\mathbf{k}\mathbf{a}_2) \cdot (\nabla + i\mathbf{k}\mathbf{a}_2)u^\pm(\varphi) - \omega^2 \varepsilon u^\pm(\varphi) = 0 \quad \text{in } S^\pm, \quad (3a)$$

$$u^\pm(\varphi) = \varphi \quad \text{on } \Gamma_0^\pm. \quad (3b)$$

Then we define the DtN operators  $\Lambda^\pm(\omega, k)$  as linear mappings of some Dirichlet data  $\varphi$  to the Neumann data of the infinite half strip solution  $u^\pm(\varphi)$  on  $\Gamma_0^\pm$

$$\Lambda^\pm(\omega, k) \varphi = \mp \partial_1 u^\pm(\cdot; \omega, k, \varphi)|_{\Gamma_0^\pm}. \quad (4)$$

With this definition of the DtN operators the linear eigenvalue problem (2) on the unbounded domain  $S$  is equivalent to a nonlinear eigenvalue problem in the defect cell  $C_0$  with DtN transparent boundary conditions on  $\Gamma_0^\pm$  [5]

$$-(\nabla + i\mathbf{k}\mathbf{a}_2) \cdot (\nabla + i\mathbf{k}\mathbf{a}_2)u - \omega^2 \varepsilon u = 0, \quad \text{in } C_0, \quad (5a)$$

$$\mp \partial_1 u = \Lambda^\pm(\omega, k) u \quad \text{on } \Gamma_0^\pm. \quad (5b)$$

### B. Characterization of the DtN operators

The DtN operators  $\Lambda^\pm(\omega, k)$  can be characterized via Dirichlet cell problems and a quadratic, operator-valued equation. To this end, let us introduce the propagation operators  $\mathcal{P}^\pm(\omega, k)$  that map some Dirichlet data  $\varphi$  on  $\Gamma_0^\pm$  to the Dirichlet data of the half strip solutions  $u^\pm(\varphi)$  of (3) on  $\Gamma_1^\pm$ , i. e.,  $\mathcal{P}^\pm(\omega, k) \varphi = u^\pm(\cdot; \omega, k, \varphi)|_{\Gamma_1^\pm}$ . These propagation operators  $\mathcal{P}^\pm(\omega, k)$  are the unique solutions of the quadratic operator-valued equations

$$\mathcal{T}_{10}^\pm(\mathcal{P}^\pm)^2 + (\mathcal{T}_{00}^\pm + \mathcal{T}_{11}^\pm)\mathcal{P}^\pm + \mathcal{T}_{01}^\pm = 0 \quad (6)$$

with eigenvalues of magnitude strictly less than one [7], which corresponds to a decay condition. Here,  $\mathcal{T}_{ij}^\pm \equiv \mathcal{T}_{ij}^\pm(\omega, k)$ ,  $i, j = 0, 1$ , are local DtN operators defined by  $\mathcal{T}_{ij}^\pm(\omega, k) \varphi = \mp (-1)^j \partial_1 u_i^\pm(\cdot; \omega, k, \varphi)|_{\Gamma_j^\pm}$  for any Dirichlet data  $\varphi$  on  $\Gamma_0^\pm$ , where  $u_i^\pm(\varphi) \equiv u_i^\pm(\cdot; \omega, k, \varphi)$ , solve the local Dirichlet cell problems

$$-(\nabla + i\mathbf{k}\mathbf{a}_2) \cdot (\nabla + i\mathbf{k}\mathbf{a}_2)u_i^\pm(\varphi) - \omega^2 \varepsilon u_i^\pm(\varphi) = 0 \quad \text{in } C_1^\pm, \\ u_i^\pm(\varphi) = \delta_{ij} \varphi \quad \text{on } \Gamma_j^\pm.$$

Then the DtN operators  $\Lambda^\pm(\omega, k)$ , defined in (4), are given by

$$\Lambda^\pm(\omega, k) = \mathcal{T}_{00}^\pm(\omega, k) + \mathcal{T}_{10}^\pm(\omega, k) \mathcal{P}^\pm(\omega, k). \quad (7)$$

## III. DISCRETIZATION

For the discretization of this problem we use high-order finite elements on quadrilaterals with curved edges as provided by the C++ library Concepts [8].

In discrete sense the operators  $\mathcal{T}_{ij}^\pm$  are matrices  $\mathbf{T}_{ij}^\pm$  whose number of columns/rows is equal to the number of degrees of freedom on the boundaries  $\Gamma_{i,j}^\pm$ . Consequently, also the propagation operators  $\mathcal{P}^\pm$  can be represented by matrices  $\mathbf{P}^\pm$  of the same size as  $\mathbf{T}_{ij}^\pm$  satisfying the quadratic, matrix-valued

equations of the form (6) and having only eigenvalues of magnitude strictly less than 1. Finally, interpreting Eq. (7) in discrete sense, the DtN operators  $\Lambda^\pm$  can be understood as matrices  $\mathbf{D}^\pm$ .

These DtN matrices  $\mathbf{D}^\pm$  are added as dense blocks to the stiffness, mass and advection matrices that correspond to the left hand side of (5a). This yields the nonlinear, matrix-valued eigenvalue problem

$$\mathbf{N}(\omega, k) \mathbf{u} = 0 \quad (8)$$

of dimension equal to the number of degrees of freedom in the defect cell  $C_0$ .

## IV. LINEARIZATION OF THE NONLINEAR EIGENVALUE PROBLEM

A sophisticated method to solve the nonlinear, matrix-valued eigenvalue problem (8) is based on a polynomial approximation using the Chebyshev interpolation and a subsequent linearization [6]. We fix the quasi-momentum  $k$  and search for eigenvalues  $\omega(k)$  of the nonlinear eigenvalue problem (8). Additionally, we have to fix an interval  $I_\omega$  of the frequency  $\omega$  where the eigenvalues  $\omega(k)$  are sought. This interval has to lie entirely inside a band gap of the PhC, since the DtN operators — and consequently the matrix-valued function  $\mathbf{N}(\omega, k)$  of the nonlinear eigenvalue problem (8) — are not analytic at band edges [4]. Analyticity of the nonlinear function is, however, a crucial prerequisite of the Chebyshev interpolation [6].

On this frequency interval  $I_\omega$  we project the  $d+1$  Chebyshev nodes  $\cos\left(\frac{i+\frac{0.5}{d+1}}{2}\right)$ ,  $0 \leq i \leq d$ , of the first kind. We will denote the projected Chebyshev nodes by  $\omega_0, \dots, \omega_d \in I_\omega$ . Introducing the first  $d+1$  Chebyshev polynomials  $c_j : I_\omega \rightarrow \mathbb{R}$ ,  $0 \leq j \leq d$ , we approximate (for fixed  $k$ )  $\mathbf{N}(\omega, k) \approx \sum_{j=0}^d \mathbf{L}_j^d c_j(\omega)$ , where the matrices  $\mathbf{L}_j^d$ ,  $0 \leq j \leq d$ , are obtained using the interpolation condition  $\mathbf{N}(\omega_i, k) = \sum_{j=0}^d \mathbf{L}_j^d c_j(\omega_i)$ ,  $0 \leq i \leq d$ . Substituting  $\mathbf{u}_j(\omega) := c_j(\omega) \mathbf{u}$ ,  $0 \leq j \leq d$ , the polynomial eigenvalue problem  $(\sum_{j=0}^d \mathbf{L}_j^d c_j(\omega)) \mathbf{u} = 0$  of order  $d$  can be linearized yielding the linear eigenvalue problem

$$\begin{pmatrix} \mathbf{0} & \mathbf{I} & & & & \\ \mathbf{I} & \mathbf{0} & \mathbf{I} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \mathbf{I} & \mathbf{0} & \mathbf{I} & \\ \mathbf{L}_0^d & \cdots & \mathbf{L}_{d-3}^d & \mathbf{L}_{d-2}^d - \mathbf{L}_d^d & \mathbf{L}_{d-1}^d & \end{pmatrix} \begin{pmatrix} \mathbf{u}_0 \\ \vdots \\ \mathbf{u}_{d-1} \end{pmatrix} \\ = \omega \begin{pmatrix} \mathbf{I} & & & & \\ & 2\mathbf{I} & & & \\ & & \ddots & & \\ & & & 2\mathbf{I} & \\ & & & & -2\mathbf{L}_d^d \end{pmatrix} \begin{pmatrix} \mathbf{u}_0 \\ \vdots \\ \mathbf{u}_{d-1} \end{pmatrix} \quad (9)$$

whose dimension is  $d$ -times larger than the original, nonlinear eigenvalue problem (8). However, thanks to the special properties of the Chebyshev interpolation, we only have to invert a matrix of the same size like the original problem, if we apply a shift and invert strategy to solve the linear eigenvalue problem, see [6] for details.

## V. BAND GAP CALCULATION

As stated in the previous section, it is crucial for the Chebyshev interpolation that the interval  $I_\omega$  lies entirely inside a band gap of the PhC. It is hence necessary to compute the band gaps for each fixed quasi-momentum  $k$ . In practice, it is common to compute so called complete band gaps, which are the intersections of the band gaps for all quasi-momenta  $k$  in the Brillouin zone  $B$ . In this work we shall instead employ an efficient algorithm to compute the  $k$ -dependent band gaps, which will allow us to compute guided modes that are not inside the complete band gaps. In other words, for each  $k \in B$  we want to determine the frequency intervals in which there only exist Bloch modes in the semi-infinite PhCs, characterized by the unit cells  $C_1^\pm$ , that decay if  $|x_i| \rightarrow \infty$ . We propose an algorithm based on Taylor expansions using high-order derivatives of the dispersion curves  $\omega(k)$ , which relies on the analyticity of  $\omega(k)$  [9]. Let us assume for simplicity that the semi-infinite PhCs on the left and right of the defect cell  $C_0$  have identical lattices and permittivities. Then we only have to do one band gap calculation and can omit the superscripts “ $\pm$ ”.

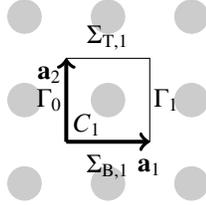


Figure 2. Sketch of the PhC with unit cell  $C_1$ , its left/right boundaries  $\Gamma_0$  and  $\Gamma_1$ , its top/bottom boundaries  $\Sigma_{T,1}$  and  $\Sigma_{B,1}$ , and its periodicity vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ .

The quasi momentum  $k$  introduced in Section I corresponds to the Floquet-Bloch transformation in the direction of  $\mathbf{a}_2$ . For the band gap calculation we consider a PhC with periodicity in both directions,  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , see Fig. 2, and hence, we apply the Floquet-Bloch transformation also in the direction of  $\mathbf{a}_1$ , which yields a quasi-momentum  $k_1 \in [-\pi/|\mathbf{a}_1|, \pi/|\mathbf{a}_1|]$ . For clarity of notation we shall therefore denote the quasi-momentum  $k$  corresponding to the Floquet-Bloch transformation in the direction of  $\mathbf{a}_2$  by  $k_2$  in this section.

Thus, the problem that we consider is: for fixed  $k_2 \in [-\pi/|\mathbf{a}_2|, \pi/|\mathbf{a}_2|]$  find  $\omega^2 \in \mathbb{R}^+$  such that there exists a real valued quasi-momentum  $k_1 \in [-\pi/|\mathbf{a}_1|, \pi/|\mathbf{a}_1|]$  and a Bloch mode  $u_{\text{PhC}}$  that satisfy

$$-(\nabla + ik_1 \mathbf{a}_1 + ik_2 \mathbf{a}_2) \cdot (\nabla + ik_1 \mathbf{a}_1 + ik_2 \mathbf{a}_2) u_{\text{PhC}} - \omega^2 \varepsilon u_{\text{PhC}} = 0 \quad (10)$$

in the unit cell  $C_1$  of the PhC with periodic boundary conditions on the top and bottom boundaries  $\Sigma_{T,1}$  and  $\Sigma_{B,1}$  as well as on the left and right boundaries  $\Gamma_0$  and  $\Gamma_1$ .

We shall directly state the discrete forms of the relevant equations. To this end, let us introduce some matrices: let  $\mathbf{M}$  denote the mass matrix in the cell  $C_1$  and let  $\mathbf{M}^\varepsilon$  be the mass matrix multiplied with the permittivity  $\varepsilon$ . Moreover, let  $\mathbf{C}_1$  denote the matrix corresponding to the term  $ik_1 \nabla \cdot \mathbf{a}_1 u_{\text{PhC}}$  in (10). Finally, we introduce the system matrix  $\mathbf{S} = \mathbf{S}(\omega, k_1, k_2)$  that corresponds to the left hand side of Eq. (10). Let  $\mathbf{u}$  denote the coefficient vector of the eigenmode  $u_{\text{PhC}}$  at  $(\omega(k_1), k_1)$ . Then,

the  $n$ -th derivative of the dispersion curve  $\omega(k_1)$  at  $(\omega(k_1), k_1)$  reads

$$\begin{aligned} \omega_{k_1}^{(n)} = & \left( n(n-1) |\mathbf{a}_1|^2 \bar{\mathbf{u}}^T \mathbf{M} \mathbf{u}_{k_1}^{(n-2)} + 2n k_1 |\mathbf{a}_1|^2 \bar{\mathbf{u}}^T \mathbf{M} \mathbf{u}_{k_1}^{(n-1)} \right. \\ & - \sum_{p=1}^{n-1} \sum_{q=0}^{n-p} \frac{n!}{p! q! (n-p-q)!} \omega_{k_1}^{(n-p-q)} \omega_{k_1}^{(q)} \bar{\mathbf{u}}^T \mathbf{M}^\varepsilon \mathbf{u}_{k_1}^{(p)} \\ & - \sum_{q=1}^{n-1} \frac{n!}{q! (n-q)!} \omega_{k_1}^{(n-q)} \omega_{k_1}^{(q)} \bar{\mathbf{u}}^T \mathbf{M}^\varepsilon \mathbf{u} \\ & \left. + i n |\mathbf{a}_1| \bar{\mathbf{u}}^T (\mathbf{C}_1 - \mathbf{C}_1^T) \mathbf{u}_{k_1}^{(n-1)} \right) \left( 2\omega \bar{\mathbf{u}}^T \mathbf{M}^\varepsilon \mathbf{u} \right)^{-1}, \end{aligned} \quad (11)$$

where the derivatives  $\mathbf{u}_{k_1}^{(n)}$  of the eigenmode  $\mathbf{u}$  at  $(\omega(k_1), k_1)$  are obtained by solving the system

$$\mathbf{S} \mathbf{u}_{k_1}^{(n)} = \mathbf{f}_n \quad (12)$$

with the vector of the right hand side

$$\begin{aligned} \mathbf{f}_n = & \sum_{p=0}^{n-1} \sum_{q=0}^{n-p} \frac{n!}{p! q! (n-p-q)!} \omega_{k_1}^{(n-p-q)} \omega_{k_1}^{(q)} \mathbf{M}^\varepsilon \mathbf{u}_{k_1}^{(p)} \\ & - i n |\mathbf{a}_1| (\mathbf{C}_1 - \mathbf{C}_1^T) \mathbf{u}_{k_1}^{(n-1)} \\ & - 2n k_1 |\mathbf{a}_1|^2 \mathbf{M} \mathbf{u}_{k_1}^{(n-1)} - n(n-1) |\mathbf{a}_1|^2 \mathbf{M} \mathbf{u}_{k_1}^{(n-2)}. \end{aligned}$$

However, note that  $\mathbf{u}_{k_1}^{(n)}$  is not determined uniquely by (12) since the eigenmode  $\mathbf{u}$  solves (12) with zero right hand side, *c.f.* Eq. (10). According to the Fredholm–Riesz–Schauder theory, for example see [10], we shall therefore add the orthogonality condition

$$\bar{\mathbf{u}}^T (\mathbf{A} + \mathbf{M}) \mathbf{u}_{k_1}^{(n)} = 0,$$

where  $\mathbf{A}$  denotes the stiffness matrix in the cell  $C_1$ .

The computation of the derivatives  $\omega_{k_1}^{(n)}$  is inexpensive since Eq. (11) involves only matrix vector multiplications of matrices that are already precomputed when solving the eigenvalue problem (10). On the other hand, the solution of (12) is inexpensive since the left hand side is identical for all orders  $n$  and hence, the matrix only needs to be inverted once.

With these derivatives at hand, we can do a piecewise, adaptive Taylor expansion of the dispersion curves. This expansion is piecewise in the sense that we only accept the expansion around a point within a trusted interval. This trusted interval is computed by estimating the remainder of the Taylor expansion and bounding it by some desired error tolerance. At the left and right boundary of the trusted interval we compute another Taylor expansion and proceed until the union of all trusted intervals covers the reduced Brillouin zone  $[0, \pi/|\mathbf{a}_1|]$ . To increase the quality of approximation we additionally do a backward check where we test if each node is recovered up to some tolerance by the Taylor expansion around the left and right boundary points of its trusted interval. If this is not the case we refine our approximation by scaling the trusted interval, for details we refer to [11]. Finally, we need to do a postprocessing of the computed data. We choose a weighted Taylor expansion where the weights of the Taylor expansions of two neighboring nodes are varied linearly between 0 to 1.

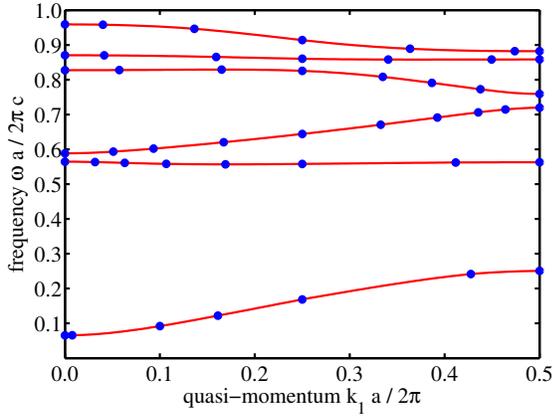


Figure 3. Band structure of TM mode in PhC with square lattice computed with Taylor expansions for fixed  $k_2 = 0.1 \cdot 2\pi$ . The blue dots show the location of the nodes for which a Taylor expansion was computed and the red lines result from a postprocessing of these expansions.

For each  $k_2$  we determine the band structure as shown exemplarily for  $k_2 = 0.1 \cdot 2\pi$  in Fig. 3, where the piecewise Taylor expansion is applied to the TM mode in a PhC with square lattice  $a = |\mathbf{a}_1| = |\mathbf{a}_2|$  with rods of radius  $0.2a$  and relative permittivity  $\varepsilon = 11.4$ .

More details on the higher-derivatives and the algorithm can be found in a forthcoming article [11].

## VI. NUMERICAL RESULTS

Let us now present numerical results of the proposed DtN method with band gap calculation using Taylor expansions and Chebyshev interpolation of the nonlinear eigenvalue problem. We will study the problem of the TM mode in a W1 PhC wave-guide with square lattice as introduced in the previous section. Fig. 4 shows the band gaps of the PhC (gray lines) that were computed using Taylor expansions. The red dots on these lines represent the guided modes computed with the Chebyshev interpolation.

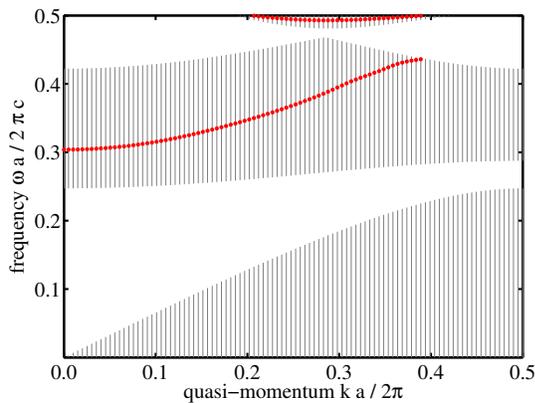


Figure 4. Band structure of TM mode in W1 PhC wave-guide with square lattice computed with DtN method using Chebyshev interpolation of order  $d = 10$ . The gray lines represent the band gaps computed using Taylor expansions, and the red dots on these lines correspond to guided modes.

Finally, we want to show convergence results. In Fig. 5 we present the mean errors of the supercell method and the

Chebyshev interpolation when applied to the computation of the guided modes in the second band gap, *c.f.* Fig. 4. As expected, we observe exponential convergence for both methods. However, the computational complexity of the supercell method increases significantly with the number of unit cells as this increases the degrees of freedom of the eigenvalue problem. On the other hand, the size of the linearized eigenvalue problem (9) of the Chebyshev interpolation also increases with the number  $d$  of Chebyshev nodes, but since this linearized eigenvalue problem can be solved using a shift and invert strategy where we only have to invert a matrix whose size is independent of  $d$ , the increase of computational complexity of the Chebyshev interpolation is less significant compared to the supercell method.

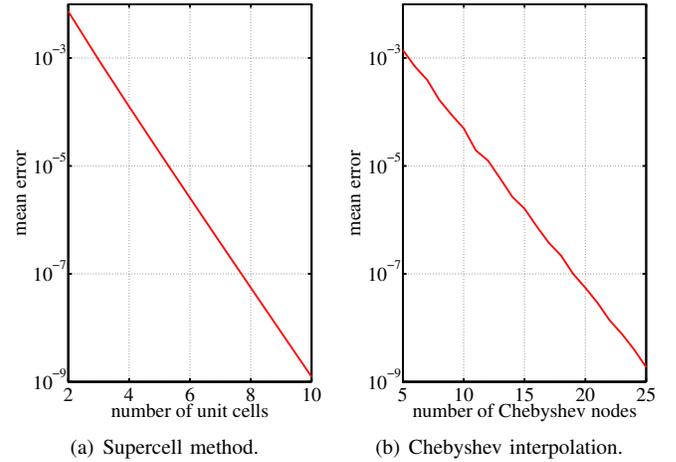


Figure 5. Mean error of the supercell method (left) with respect to the number of unit cells per half strip, and the DtN method using Chebyshev interpolation (right) with respect to the number of Chebyshev nodes.

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