Weierstraß-Institut für Angewandte Analysis und Stochastik Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint

ISSN 2198-5855

Solving a spectral problem for large-area photonic crystal surface-emitting lasers

Mindaugas Radziunas¹, Eduard Kuhn¹, Hans Wenzel²

submitted: November 28, 2023

 Weierstrass Institute Mohrenstraße 39 10117 Berlin Germany E-Mail: mindaugas.radziunas@wias-berlin.de eduard.kuhn@wias-berlin.de ² Ferdinand-Braun-Institut Leibniz Institut für Höchstfrequenztechnik Gustav-Kirchhoff-Straße 4 12489 Berlin Germany E-Mail: hans.wenzel@fbh-berlin.de

No. 3059 Berlin 2023



2020 Mathematics Subject Classification. 78M20, 78A60, 78-04, 35L02, 65N25, 65Y04.

Key words and phrases. Modeling, finite difference, spectral problem, Green's function, exponential growth, simulations, semiconductor laser, photonic crystal.

This work was performed in the frame of the project "PCSELence" (K487/2022) funded by the German Leibniz Association. We are indebted to P. Crump and B. King (FBH) for initiating this study.

Edited by Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS) Leibniz-Institut im Forschungsverbund Berlin e. V. Mohrenstraße 39 10117 Berlin Germany

Fax:+493020372-303E-Mail:preprint@wias-berlin.deWorld Wide Web:http://www.wias-berlin.de/

Solving a spectral problem for large-area photonic crystal surface-emitting lasers

Mindaugas Radziunas, Eduard Kuhn, Hans Wenzel

Abstract

We present algorithms for constructing and resolving spectral problems for novel photonic crystal surface-emitting lasers with large emission areas, given by first-order PDEs with two spatial dimensions. These algorithms include methods to overcome computer-arithmetic-related challenges when dealing with huge and small numbers. We show that the finite difference schemes constructed using relatively coarse numerical meshes enable accurate estimation of several major optical modes, which are essential in practical applications.

1 Introduction

Semiconductor lasers (SLs) are small, efficient, relatively long-living, and cheap devices used in many modern applications. SLs are applied, for example, in instruments and sensors requesting an enhanced coherence of light, optical communication systems demanding regular and stationary or irregular dynamics, or for material processing requiring up to a few kilowatt optical power. The emission of conventional high-power edge-emitting lasers considered in our previous works [10, 13], for example, is mainly concentrated within the rectangular area at the laser facet. The beam divergence in vertical and lateral directions is different, so that the use of additional optical elements (lenses) for collimating the emitted fields is unavoidable. However, even sophisticated external optics can not improve the poor lateral beam quality induced by multiple lateral optical modes contributing to the overall emission of broad area lasers [12].



Figure 1: Schematics of photonic-crystal surface-emitting semiconductor laser. (a): sandwiching of material layers along vertical ($z \in [0, Z]$) direction. (b): three-dimensional scheme of the device. (c): lateral ($(x, y) \in [0, L] \times [0, L]$) photonic crystal layer consisting of three vertically-homogeneous sublayers. (d): structure of the elementary cell of lateral size $a \times a$ within each sublayer of the crystal.

In 1999, Prof. Susumu Noda and his group from Kyoto University proposed a Photonic-Crystal (PC) surface-emitting laser (SEL) [5], see schematic representation of PCSEL in Fig. 1. The operation of this device is determined by the vertical structure of the SL (panels (a), (b)), the size and configuration of

the PC layers (panel (c)), and the structure of unit cells of the PC (panel (d)). Whereas the vertical configuration should support a single *vertical* transverse-electric optical mode, the PC structure provides diffraction of the field in both lateral directions and its redirection towards the vertical output facet of the laser. Currently, the emission power of the best PCSELs [11] is comparable to that of the best edge emitters. In contrast to high-power edge-emitting SLs, high-power PCSELs have much lower power density at the output facet (damaging the facet coating is less probable) and possess radial symmetry and low emission divergence. On the other hand, best PCSELs rely on the PCs composed of periodically made air holes within semiconductor layers, i.e., technology that is more elaborated compared to standard all-semiconductor layer growth-etching-regrowth procedures. Compared to semiconductorair PCs, coupling of the different components of the optical fields by diffraction in all-semiconductor PC layers is weaker, which requires an increase of the lateral dimension of PCSEL (increasing factor L in Fig. 1(c)) and, thus, the development of advanced algorithms and numerical schemes suited for solving PCSEL models within a large lateral domain $(x, y) \in [0, L] \times [0, L]$. Construction and study of currently available PCSEL models for large-area devices and solving the related spectral problem is the main aim of this work.

Our paper is structured as follows. In Section 2, we introduce a spectral problem for PCSELs, a system of first-order partial differential equations for slowly varying complex components of an optical mode in a two-dimensional spatial domain. We also present several nontrivial auxiliary problems that should be solved to define the parameters entering the model equation. Section 3 is devoted to constructing the complex 4×4 dimensional matrix providing coupling of counter- and cross-propagating fields. In particular, numerical algorithms are provided, and several challenges related to using huge and almost vanishing numbers are discussed. Section 4 discusses numerical methods for solving the spectral problem. Here, we construct, apply, and analyze finite difference schemes of different precision. We show that the schemes constructed using coarse numerical meshes can provide acceptable precision for a few primarily important optical modes. Some conclusions are drawn in Section 5.

2 Mathematical model

2.1 Optical field equations and optical modes

To describe the spatio-temporal dynamics in PCSELs, we use the three-dimensional coupled-wave model derived from the Maxwell equations by making some assumptions [7, 6]. Neglecting noise terms, the central part of this model, a system of the first-order PDEs in two lateral dimensions for slowly varying field amplitudes $u(x, y, t) = (u^+, u^-)^T$ and $v(x, y, t) = (v^+, v^-)^T$ (^T denotes the transpose), can be written as

$$\frac{1}{v_g}\frac{\partial}{\partial t} \begin{pmatrix} u\\v \end{pmatrix} = \left[i\mathbf{C} - \begin{pmatrix} \sigma\frac{\partial}{\partial x} & \mathbf{0}\\ \mathbf{0} & \sigma\frac{\partial}{\partial y} \end{pmatrix} - i\Delta\beta \right] \begin{pmatrix} u\\v \end{pmatrix}, \quad (x,y) \in [0,L] \times [0,L],$$
boundary conditions: $u^+|_{x=0} = u^-|_{x=L} = v^+|_{y=0} = v^-|_{y=L} = 0.$
(1)

Here, L defines the lateral dimensions of the PCSEL, $v_g = c_0/n_g$ is the group velocity (c_0 : speed of light in vacuum, n_g : group index), $\sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, **0** is a 2×2 zero matrix, whereas **C** is a nontrivial 4×4 field coupling matrix, which will be discussed in detail in the second part of this Section. Finally, $\Delta\beta = \Delta\beta(N;T)$ is a carrier N- and temperature T-dependent relative propagation factor, see, e.g., Ref. [13]. Its real part represents changes in the refractive index and, thus, deviation of the lasing frequency (or wavelength) from the reference frequency (wavelength λ_0). The imaginary part is defined

by (*N*-dependent) optical amplification and losses within the PCSEL. The dependence of $\Delta\beta$ on self-heating in high-power SLs is essential. However, due to significantly differing time scales of the photon, carrier, and temperature dynamics, temperature T(x, y, t) remains nearly unchanged within typically calculated time windows and should be accounted for parametrically [13]. On the contrary, temporal and spatial changes of the carriers N(x, y, t) in dynamical simulations are crucial, such that one has to supplement the model with equations governing the carrier dynamics; see, e.g., Refs. [6, 12]. If the current injected into a laser is switched on, N grows, causes changes of $\Delta\beta$, and, most importantly, implies growth of $\Im\Delta\beta$ until it reaches some threshold where the laser is switched on. After this lasing threshold is reached, (averaged) N and $\Delta\beta$ remain approximately fixed, whereas further growth of electrical pumping induces growth of the emission's power. In the present paper, we are mainly interested in the study of the threshold behavior of PCSELs, where $\Delta\beta$ remains (nearly) uniform in space and stationary in time, thus can be well represented by a single complex constant $\overline{\Delta\beta}$.

For any fixed in time $\Delta\beta$, the field equations (1) define optical modes $(\Omega, \Phi(x, y))$. The four-component vector-eigenfunction $\Phi(x, y)$ provides spatial distributions of four field components. The real and imaginary parts of the complex frequency Ω represent the mode's relative frequency and damping, respectively. These modes can be found by substituting the Ansatz

$$\begin{pmatrix} u(x,y,t)\\v(x,y,t) \end{pmatrix} = \Phi(x,y)e^{i\Omega t}, \quad \Phi = \begin{pmatrix} \Phi_u\\\Phi_v \end{pmatrix}, \quad \Phi_\nu = \begin{pmatrix} \Phi_\nu^+\\\Phi_\nu^- \end{pmatrix}, \quad \nu \in \{u,v\}$$
(2)

into Eqs. (1) and resolving the resulting spectral problem

$$\begin{bmatrix} i\mathbf{C} - \begin{pmatrix} \sigma \frac{\partial}{\partial x} & \mathbf{0} \\ \mathbf{0} & \sigma \frac{\partial}{\partial y} \end{pmatrix} - \Lambda \end{bmatrix} \Phi = 0, \quad (x, y) \in [0, L] \times [0, L], \\ \Lambda = i(\overline{\Delta\beta} + \frac{\Omega}{v_g}), \quad \Phi_u^+(0, y) = \Phi_u^-(L, y) = \Phi_v^+(x, 0) = \Phi_v^-(x, L) = 0.$$
(3)

Here, we exploit our assumption of spatially uniform distribution of $\Delta\beta = \overline{\Delta\beta}$, which allows combining the complex optical frequency Ω and the complex factor $\overline{\Delta\beta}$ into a single complex eigenvalue Λ . $-\Re\Lambda$ represents the threshold of the mode, i.e., the value of $\Im\overline{\Delta\beta}$ at which the mode damping $\Im\Omega$ vanishes.

The spectral problem (3) defines multiple optical modes (Λ, Φ) and is vital when designing PCSEL devices. Mode with the largest but still negative $\Re\Lambda$ (the main mode) is excited first when up-tuning the bias current, which causes an increase of $\Im\overline{\Delta\beta}$. The damping $\Im\Omega$ of this mode vanishes; a threshold of this mode is the lasing threshold, $-\Re\Lambda_1 = [\Im\Delta\beta]_{\rm th}$; the remaining modes have negative $\Im\Omega$, i.e., $\Re\Lambda_{\rm rest} < \Re\Lambda_1$, and remain damped. For practical applications, PCSEL configurations should exhibit small $[\Im\Delta\beta]_{\rm th}$, i.e., large $\Re\Lambda_1$, and a possibly large threshold gap to other modes, i.e. large $\Re(\Lambda_1 - \Lambda_{\rm rest})$, which allows expecting a single-mode operation of the PCSEL. Besides, when analyzing separate modes, one can be interested in the balance of the generated intensity, losses within and at the lateral edges of the PCSEL, and radiation in the vertical to PC and QW layers direction. Eq. (3) allows relating integral factors \mathcal{I}_l (losses at the lateral borders), \mathcal{I}_g , and \mathcal{I}_v (mainly determined by the generated and vertically radiated field intensity but also include field losses inside the PCSEL) [7].

Lemma 1. Let Λ and the nontrivial four-component vector-function $\Phi(x, y)$ satisfy Eq. (3). Then the following integral balance relations hold:

$$\mathcal{I}_{g} = \mathcal{I}_{v} + \mathcal{I}_{l}, \quad \text{where} \quad \mathcal{I}_{g} = -2\Re\Lambda \|\Phi\|^{2}, \quad \mathcal{I}_{v} = 2\Im(\Phi, \mathbf{C}\Phi),$$

$$\mathcal{I}_{l} = \int_{0}^{L} |\Phi_{u}^{+}(L, y)|^{2} + |\Phi_{u}^{-}(0, y)|^{2} dy + \int_{0}^{L} |\Phi_{v}^{+}(x, L)|^{2} + |\Phi_{v}^{-}(x, 0)|^{2} dx.$$
(4)

Here $(\xi, \zeta) = \int_0^L \int_0^L \sum_{j=1}^{\dim\{\xi,\zeta\}} \xi_j^*(x, y) \zeta_j(x, y) dx dy$ is the scalar product of vector-functions ξ and ζ , and $\|\xi\| = (\xi, \xi)^{1/2}$ is a corresponding norm of ξ .

Proof. The relations (4) can be obtained after scalar multiplication of both sides of Eq. (3) by 2Φ and taking the real part of the resulting equation.

2.2 Coupling of the optical fields

The coupling matrix C depends on the laser's vertical structure, see Fig. 1(a)-(c), the PC unit cells' size and shape, Fig. 1(d), and the real squared refractive index $\bar{n}^2(x, y, z)$, which is a part of the complex dielectric constant $\bar{\epsilon}(x, y, z) = \bar{n}^2(x, y, z) + \Delta \epsilon(x, y, z)$ in each material layer, Fig. 1(a). Here, complex $\Delta \epsilon$ accounts for the material's field absorption and carrier- and temperature-induced corrections of the dielectric constant. A desired operation of PCSELs can be achieved only for devices with $\lambda_0 \approx a n_{\bullet}$ (a: the size of the PC unit cell, n_{\bullet} : effective refractive index of the main vertical optical mode). This work presents the basic steps of the algorithm used to construct C. Refs. [7, 6] provide more physical insight into this derivation.

The PCSEL device is sandwiched from m vertically homogeneous material layers \bar{S}_k along the vertical coordinate z, see Fig. 1(a). Let

$$\bar{S}_{k} = [z_{k-1}, z_{k}], \ S_{k} = (z_{k-1}, z_{k}), \ S_{0} = (-\infty, 0), \ S_{m+1} = (Z, +\infty),
\cup_{k=1}^{m} \bar{S}_{k} = [0, Z], \ |S_{k}| = z_{k} - z_{k-1}, \ \bar{z}_{k} = \frac{z_{k-1} + z_{k}}{2},$$
(5)

where $z_0 = 0$, $z_m = Z$, and other z_k are interfaces of corresponding layers. Each layer is either laterally homogeneous with a real refractive index $n_k \equiv \bar{n}(x, y, z)|_{z \in S_k}$ or is a PC layer determined by the pair of real indices (n_k^I, n_k^{II}) representing the material within the PC feature (e.g., air with $n_k^{II} \approx 1$ as in [7, 6]) and surrounding semiconductor material, respectively. By n_k^2 here, we denote the spatial average of $\bar{n}^2(x, y, z)|_{z \in S_k}$ over the unit cell of the PC,

$$n_k^2 = \frac{1}{a^2} \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} \bar{n}^2(x, y, z)|_{z \in S_k} dx dy.$$
(6)

The real positive piece-wise function n(z), $n(z)|_{z \in S_k} = n_k$, k = 1, ..., m, represents the (laterallyaveraged) refractive index of each material layer, including PC layers. If considered, real refractive indices of the infinitely broad lower (S_0) and upper (S_{m+1}) materials surrounding the PCSEL device are denoted as n_L and n_U , respectively. In this work, we assume it is air, i.e., $n_{L,U} \approx 1$. Constants $n_{L,U}$ and the function n(z) define the layer-wise constant function $\sigma(z)$ and factors $\sigma_{L,U}$,

$$\sigma(z)|_{z\in S_j} = \sigma_j \stackrel{def}{=} \tilde{\sigma}(n_{\bullet}, n_j), \quad j = \{1, \dots, m\}, \quad \sigma_{L,U} \stackrel{def}{=} \tilde{\sigma}(n_{\bullet}, n_{L,U}),$$

where $\tilde{\sigma}(\xi, \zeta) = k_0 \sqrt{\xi^2 - \zeta^2} \in \mathbb{C}, \quad \Re \tilde{\sigma}(\xi, \zeta) \ge 0, \quad k_0 \stackrel{def}{=} \frac{2\pi}{\lambda_0},$ (7)

exploited in the one-dimensional Helmholtz problem

$$\frac{d^2}{dz^2}\Theta(z) - \sigma^2(z)\Theta(z) = 0, \qquad z \in [0, Z], \quad \sigma^2(z) \in \mathbb{R},$$
(8)

satisfying homogeneous Dirichlet ($\rho = 0$) or natural radiating ($\rho = 1$) boundary conditions (BCs) at z = 0 and z = Z:

$$\rho \frac{d\Theta}{dz}(0) = \sigma_L \Theta(0), \ \rho \frac{d\Theta}{dz}(Z) = -\sigma_U \Theta(Z), \ \sigma_{L,U} \in \mathbb{R}, \ \sigma_{L,U} \ge 0.$$
(9)

Within each S_k , function $\Theta(z)$ can be written as a linear combination of two special solutions $\theta_k^+(z)$ and $\theta_k^-(z)$ to a linear homogeneous Eq. (8):

$$\Theta(z)|_{z \in S_k} = \mathcal{B}_k^{\Theta T} \theta_k(z), \quad \mathcal{B}_k^{\Theta} \stackrel{def}{=} \begin{pmatrix} \Theta(z_k) \\ \Theta(z_{k-1}) \end{pmatrix}, \quad \theta_k = \begin{pmatrix} \theta_k^+ \\ \theta_k^- \end{pmatrix},$$

$$\theta_k^{\pm}|_{z \in S_k} \text{ satisfy Eq. (8)}, \quad \theta_k(z_k) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \theta_k(z_{k-1}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

$$(10)$$

DOI 10.20347/WIAS.PREPRINT.3059

Eqs. (8), (9) with σ determined in Eq. (7) define the real effective refractive index $n_{\bullet} \in [\max\{n_L, n_U\}, \max_z n(z)]$ (or $(0, \max_z n(z)]$ in the case of Dirichlet BCs) and the corresponding nontrivial vertical mode $\Theta(z)$, normalized by $\int_{\mathbb{R}} |\Theta(z)|^2 dz = 1$. In typical applications, n_{\bullet} is between 3 and 4, such that BCs (9) for $\rho = 1$ and $n_{U,L} \approx 1$ represent at $z \to \pm \infty$ vanishing optical fields. Non-vanishing Fourier expansion coefficients within the PC layers S_j ,

$$\xi_{r,s}^{j} = \frac{1}{a^{2}} \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} \bar{n}^{2}(x,y,z)|_{z \in S_{j}} e^{i2\pi(rx+sy)/a} dx dy, \quad r,s \neq 0,$$
(11)

together with the PC-layer-wise integrals

$$\mathcal{P}_{j}^{\Theta} = \int_{S_{j}} |\Theta(z)|^{2} dz = \mathcal{B}_{j}^{\Theta T} \mathbf{p}_{j} \mathcal{B}_{j}^{\Theta^{*}}, \quad \mathbf{p}_{j} \stackrel{def}{=} \int_{S_{j}} \theta_{j}(z) \theta_{j}^{*T}(z) dz,$$

$$\mathcal{G}_{(r,s)}^{(k,j)} = \int_{S_{k}} \int_{S_{j}} G_{(r,s)}(z, z') \Theta(z') dz' \Theta^{*}(z) dz = \mathcal{B}_{j}^{\Theta T} \mathbf{g}_{k,j} \mathcal{B}_{k}^{\Theta^{*}},$$

$$\mathbf{g}_{(r,s)}^{(k,j)} \stackrel{def}{=} \int_{S_{k}} \int_{S_{j}} \theta_{j}(z') G_{(r,s)}(z, z') dz' \theta_{k}^{*T}(z) dz,$$
(12)

determined by the values of Θ at material interfaces and (2×2) matrices \mathbf{p}_j and $\mathbf{g}_{(r,s)}^{(k,j)}$, are used to define \mathbf{C} . Green's functions $G_p(z, z')$ with $p \stackrel{def}{=} (r, s)$ and $|p|^2 \stackrel{def}{=} r^2 + s^2$ solve the inhomogeneous problem [8]

$$\frac{\partial^2}{\partial z^2} G_p(z, z') - \sigma_p^2(z) G_p(z, z') = -\delta(z - z'), \ (z, z') \in [0, Z] \times [0, Z],$$
(13)

with radiating boundary conditions

$$\frac{\partial G_p(0,z')}{\partial z} = \sigma_{p,L} G_p(0,z'), \qquad \frac{\partial G_p(Z,z')}{\partial z} = -\sigma_{p,U} G_p(Z,z'). \tag{14}$$

 $\delta(\zeta)$ in Eq. (13) is the Dirac's delta-function, whereas σ_p is defined by

$$\sigma_p(z) = \tilde{\sigma}(\frac{|p|\lambda_0}{a}, n(z)), \ \sigma_{p,j} = \tilde{\sigma}(\frac{|p|\lambda_0}{a}, n_j), \ j \in \{1, \dots, m\} \cup \{L, U\}.$$
(15)

Since $\frac{\lambda_0}{a} \approx n_{\bullet}$, for |p| = 1 (not used when building C), the left-hand side of Eq. (13) reminds that of Eq. (8). At $z = z' \pm 0$, Eq. (13) implies

$$G_p(z'+0,z') = G_p(z'-0,z'), \quad \frac{\partial G_p(z'+0,z')}{\partial z} = \frac{\partial G_p(z'-0,z')}{\partial z} - 1.$$
(16)

In typical applications, for |p| > 1, the factors $\sigma_{p,j}$ are strictly positive real, such that BCs (14) imply the convergence of $|G_p(z, z')|$ to zero when $z \to \pm \infty$. When |p| = 0, the real parts of $\sigma_{p,L}$ and $\sigma_{p,U}$ are absent, such that the radiated fields preserve their intensity outside the domain [0, Z]. In this case, we use $\sigma_{p,\{L,U\}} = ik_0|n_{\{L,U\}}|$, which reminds us of Sommerfeld's radiation conditions, even though those are formulated only for two- and three-dimensional cases.

Matrix C is defined as an infinite sum of simpler 4×4 -dimensional matrices, which are functions of $\mathcal{G}_{(r,s)}$, \mathcal{P}^{Θ} , and $\xi_{r,s}$:

$$\mathbf{C} = \mathbf{C}_{1D}(\mathcal{P}^{\Theta}, \xi_{\pm 2,0}, \xi_{0,\pm 2}) + \mathbf{C}_{rd}(\mathcal{G}_{(0,0)}, \xi_{\pm 1,0}, \xi_{0,\pm 1}) + \mathbf{C}_{2D}, \mathbf{C}_{2D} = \sum_{|r|+|s|>1} \mathbf{C}_{2D}^{(r,s)}(\mathcal{G}_{(r,s)}, \mathcal{P}^{\Theta}, \xi_{r\pm 1,s}, \xi_{r,s\pm 1}).$$
(17)

 C_{rd} is responsible for the outcoupling of the radiated light. For considered real-valued \bar{n}^2 , C_{1D} is a Hermitian matrix, inducing coupling of counter propagating fields only, whereas another Hermitian matrix C_{2D} incorporates all higher-order effects, including cross-coupling of fields, which is necessary for achieving high quality of radiation. For more details on the definition of C, see Refs. [7, 6].

Remark 1. Since C_{1D} and C_{2D} in Eq. (17) are Hermitian, i.e., $C - C^{*T} = C_{rd} - C_{rd}^{*T}$, the integral factor \mathcal{I}_v in Eq. (4) can be reformulated as

$$\mathcal{I}_{v} = 2\Im(\Phi, \mathbf{C}\Phi) = -(\Phi, i[\mathbf{C} - \mathbf{C}^{*T}]\Phi) = 2\Im(\Phi, \mathbf{C}_{\mathrm{rd}}\Phi),$$
(18)

i.e., is determined only by the radiative component of the matrix C.

The main numerical cost in estimating C is calculations of the double integrals $\mathcal{G}_{(r,s)}^{(k,l)}$ in Eq. (12) for large sets of parameters (r, s). Estimation of these integrals using numerically discretized functions $\Theta(z)$ and $G_{(r,s)}(z, z')$ is inefficient, especially when |p| is large, which causes a very fast exponential growth and decay of $|G_{(r,s)}(z, z')|$ at $z \approx z'$. Luckily, provided n_{\bullet} is known, θ and $G_{(r,s)}$ can be written as linear combinations of exponentials¹

$$\begin{cases} e^{\sigma_j(z-\bar{z}_j)}, \ e^{-\sigma_j(z-\bar{z}_j)} & \text{for } \theta_j(z) \text{ in } S_j \\ e^{\nu\sigma_{p,k}(z-\bar{z}_j)} e^{\nu'\sigma_{p,j}(z'-\bar{z}_j)}, \ \nu,\nu' \in \pm & \text{for } G_p^{(k,j)}(z,z') \text{ in } S_k \times S_j \end{cases},$$
(19)

and the matrices \mathbf{p}_j , $\mathbf{g}_p^{(k,j)}$ in Eq. (12) admit analytic expressions relying on their integrals. Still, these expressions rely on possibly huge and almost vanishing exponentials $e^{\sigma_{\cdot,j}|S_j|}$ and corresponding \sinh and \cosh functions, which can not be properly handled by computer arithmetics. To avoid numerical problems even when $\sigma_j \to 0$ (not a very probable case in realistic problems, achievable only when $n_{\bullet} = n_j$) or $e^{\sigma_{\cdot,j}|S_j|} \to \infty$ (unavoidable in calculations of Green's function with large |p| and large positive σ), we introduce new notations:

$$(1 - \Gamma_j) \stackrel{def}{=} \frac{2e^{-\sigma_j |S_j|}}{1 + e^{-\sigma_j |S_j|}}, \qquad \Gamma_j = 1 - (1 - \Gamma_j) = \tanh \frac{\sigma_j |S_j|}{2},$$

such that $\Re \Gamma_j \ge 0, \quad \Gamma_j \stackrel{\sigma_j \to 0}{\longrightarrow} 0, \quad \frac{\Gamma_j}{\sigma_j} \stackrel{\sigma_j \to 0}{\longrightarrow} \frac{|S_j|}{2}, \quad \Gamma_j \stackrel{\Re \sigma_j |S_j| \gg 1}{\longrightarrow} 1.$ (20)

In practical calculations, we define first $1 - \Gamma_j$ (almost zero when $\Gamma_j \approx 1$) and only then Γ_j and the remaining Γ_j -dependent expressions. In this way, we can keep a tiny but still non-vanishing factor $1 - \Gamma_j$, which could otherwise be lost due to computer arithmetics².

3 Construction of the coupling matrix C

3.1 Transfer matrices

When deriving the matrix C, we consider Eqs. (8) and (13), both related to the ordinary differential equation

$$F''(z) - \sigma^2(z)F(z) = 0, \qquad z \in \bigcup_{j=1}^m S_j,$$
 (21)

where $\sigma(z)$ is a complex layer-wise constant function,

$$\sigma(z)|_{z\in S_j} = \sigma_j \in \mathbb{C}, \quad \sigma_j^2 \in \mathbb{R}, \quad \Re \sigma_j \ge 0, \quad j \in \{1, \dots, m\}.$$
(22)

Below, we give several formulas for translating F and F' between spatial positions z and z' by transfer matrices [2] and present algorithms for avoiding possibly huge exponentials $|e^{\sigma_j|S_j|}|$ in calculations. These formulas and algorithms are used for constructing the vertical mode function $\Theta(z)$, Green's functions $G_p(z, z')$, and required integral expressions of these functions.

¹In general, it is possible that $n_{\bullet} = n_k$ in specific layers S_k , such that $\sigma_k = 0$, and instead of exponentials (19), we have to use linear w.r.t. *z* functions. In most cases, the formulas derived below for nonzero σ_k can be corrected by taking their limit with $\sigma_k \to 0$. Factors $\sigma_{p,k}$ used to construct Green's functions are never zero in real applications.

²For example, $e^{-2\sigma_j|S_j|}$ can be of order 10^{-100} and still be treated correctly in multiplicative expressions in the computer code. However, nominally the same number $(e^{-2\sigma_j|S_j|} + 1) - 1$ can be treated as zero during the calculations.

Lemma 2. Assume that $F(z) \in C^2(S_j)$ satisfies Eqs. (21), (22), and \mathcal{B}_j^F (i.e., $F(z_{j-1})$ and $F(z_j)$) are known. Then, according to Eq. (10),

$$F(z) = \mathcal{B}_j^{FT} \theta_j(z), \text{ where } \theta_j = \begin{pmatrix} \theta_j^+ \\ \theta_j^- \end{pmatrix}, \ \theta_j^{\pm}(z) = \frac{\pm \sinh \sigma_j (z - \bar{z}_j \pm |S_j|/2)}{\sinh \sigma_j |S_j|}.$$
 (23)

If instead of $F(z_j)$ (or $F(z_{j-1})$) we have $F'(z_{j-1})$ (or $F'(z_j)$), the vector $\binom{F}{F'}(z)$ at any $z \in S_j$ can be written using transfer matrices:

$$\binom{F}{F'}(z) = \mathbf{M}_{j}(z, z_{j-1}; \sigma_{j}) \binom{F}{F'}(z_{j-1}) = \mathbf{M}_{j}(z, z_{j}; \sigma_{j}) \binom{F}{F'}(z_{j}),$$

$$\mathbf{M}_{j}(z, \tilde{z}; \sigma_{j})|_{z,\tilde{z}\in\bar{S}_{j}} \stackrel{def}{=} \binom{\cosh(\sigma_{j}(z-\tilde{z}))}{\sigma_{j}\sinh(\sigma_{j}(z-\tilde{z}))} \frac{\sinh(\sigma_{j}(z-\tilde{z}))/\sigma_{j}}{\cosh(\sigma_{j}(z-\tilde{z}))}.$$

$$(24)$$

When $\sigma_j \to 0$, expressions $\frac{\sinh \sigma_j \xi}{\sinh \sigma_j |S_j|}$ within $\theta_j(z)$ in Eq. (23) should be replaced by $\frac{\xi}{|S_j|}$, and $\mathbf{M}_j(z, \tilde{z}; \sigma_j)$ in (24) by the matrix $\begin{pmatrix} 1 & z-\tilde{z} \\ 0 & 1 \end{pmatrix}$.

Proof. One can easily check that the expressions for $\theta_j(z)$ in (23) and F(z) in (24) satisfy Eq. (21), whereas at the edges of S_j , $\theta_j(z)$ fulfills Eq. (10). Since the second-row elements of \mathbf{M}_j in (24) are *z*-derivatives of the corresponding first-row elements, \mathbf{M}_j provides a correct expression of F'(z) along S_j . The expressions for $\sigma_j \to 0$ follow directly from the relation $\lim_{\xi \to 0} \frac{\sinh \xi}{\xi} = 1$.

Remark 2. Transfer matrices are invertible, $\mathbf{M}_j(z, \tilde{z}; \sigma_j) = \mathbf{M}_j^{-1}(\tilde{z}, z; \sigma_j)$, and can be combined with each other, $\mathbf{M}_j(z, \tilde{z}; \sigma_j) = \mathbf{M}_j(z, z'; \sigma_j)\mathbf{M}_j(z', \tilde{z}; \sigma_j)$. In both these cases we assume that $z, z', \tilde{z} \in \bar{S}_j$.

Corollary 1. A complex conjugate of F(z) satisfying all conditions of Lemma 2 is given by Eq. (23) using $\mathcal{B}_i^{F^*}$ instead of \mathcal{B}_i^F .

Proof. We can easily show that the vector-function $\theta_j(z)$ in Eq. (23) is real, which immediately proves our statement. Recall that $\sigma_j^2 \in \mathbb{R}$. For $\sigma_j^2 > 0$, we have $\sigma_j > 0$ and $\frac{\sinh \sigma_j \xi}{\sinh \sigma_j |S_j|} \in \mathbb{R}$. When $\sigma_j^2 < 0$, $\sigma_j = i |\sigma_j|$ and the same expressions can be written as $\frac{\sin |\sigma_j|\xi}{\sin |\sigma_j||S_j|} \in \mathbb{R}$.

Corollary 2. Matrix p_j introduced in Eq. (12) can be written as

$$\mathbf{p}_{j} \stackrel{def}{=} \begin{pmatrix} p_{j}^{+} & p_{j}^{-} \\ p_{j}^{-} & p_{j}^{+} \end{pmatrix}, \quad p_{j}^{\pm} = \frac{2[\Gamma_{j}^{2} \pm 1] + [\Gamma_{j}^{2} \mp 1](1 - \Gamma_{j}^{2})|S_{j}|\frac{\sigma_{j}}{\Gamma_{j}}}{8\sigma_{j}\Gamma_{j}} \xrightarrow{\sigma_{j} \to 0} \frac{(3\pm 1)|S_{j}|}{12}.$$

$$(25)$$

Proof. According to Corollary 1, θ_j defined in Eq. (23) is real, i.e., $\theta_j = \theta_j^*$. Integration of $\theta_j^+ \theta_j^-$, $(\theta_j^+)^2$, and $(\theta_j^-)^2$ over S_j imply expressions (25). The limit of these expressions for $\sigma_j \to 0$ can be found using L'Hopital's rule.

Lemma 3. Assume that the complex function $F(z) \in C^2(\bigcup_{j=1}^m S_j) \cup C^1([0, Z])$ satisfies the problem (21), (22). Then, we can construct composite transfer matrices $\mathbf{M}(z_l, z_k; \sigma)$, translating the vector $\binom{F}{F'}(z)$ between any layer interfaces z_k and z_l , $0 \leq k, l \leq m$. If $\{S_j\}$ are all layers between z_k and z_l , the composite matrix elements can be written as linear combinations of all different products of exponentials $e^{\pm \sigma_j |S_j|}$.

Proof. For simplicity, let us assume that $z_l > z_k$, such that $\{S_j\}$ are all layers with indices $j = k + 1, \ldots, l$. Because of the continuity of F and F', transfer matrices (24) can also be used at the layer borders, which also are borders of the neighboring layer S_{j-1} or S_{j+1} . By superposing layer-wise transfer matrices \mathbf{M}_j , we construct the required overall transfer matrix,

$$\mathbf{M}(z_l, z_k; \sigma) = \mathbf{M}_l(z_l, z_{l-1}; \sigma_l) \cdots \mathbf{M}_{k+1}(z_{k+1}, z_k; \sigma_{k+1}),$$
(26)

propagating $\binom{F}{F'}(z)$ from z_k to z_l . Each of submatrices \mathbf{M}_j is determined by combinations of $e^{-\sigma_j|S_j|}$ and $e^{+\sigma_j|S_j|}$ (or just constants 0, 1, $|S_j|$ if $\sigma_j \to 0$). Thus, the elements of the overall matrix are as suggested in this Lemma. An invertibility of each \mathbf{M}_j , see Remark 2, allows us to construct an inverse matrix $\mathbf{M}^{-1}(z_l, z_k; \sigma) = \mathbf{M}(z_k, z_l; \sigma) = \mathbf{M}_{k+1}(z_k, z_{k+1}; \sigma_{k+1}) \cdots \mathbf{M}_l(z_{l-1}, z_l; \sigma_l)$.

Corollary 3. We can rewrite matrices $\mathbf{M}(z_l, z_k; \sigma)$ with $k \neq l$ in Eq. (26) as

$$\mathbf{M}(z_{l}, z_{k}; \sigma) = \left[\prod_{j=\min\{l,k\}}^{\max\{l,k\}} e^{\sigma_{j}|S_{j}|} \right] \mathbf{M}_{[l,k]}^{\dagger \operatorname{sgn}(l-k)}(\sigma),$$

$$\mathbf{M}_{[l,k]}^{\dagger \nu}(\sigma) = \begin{cases} \mathbf{M}_{[l]}^{\dagger \nu}(\sigma_{l}) \cdots \mathbf{M}_{[k+1]}^{\dagger \nu}(\sigma_{k+1}) & \text{for } \nu = + \\ \mathbf{M}_{[l+1]}^{\dagger \nu}(\sigma_{l+1}) \cdots \mathbf{M}_{[k]}^{\dagger \nu}(\sigma_{k}) & \text{for } \nu = - \end{cases}, \quad \text{where}$$

$$\mathbf{M}_{[j]}^{\dagger \pm}(\sigma_{j}) \stackrel{def}{=} \frac{1}{(1+\Gamma_{j})^{2}} \begin{pmatrix} 1+\Gamma_{j}^{2} \ \pm 2\Gamma_{j}/\sigma_{j} \\ \pm 2\sigma_{j}\Gamma_{j} \ 1+\Gamma_{j}^{2} \end{pmatrix} \stackrel{\sigma_{j} \to 0}{\longrightarrow} \begin{pmatrix} 1 \ \pm |S_{j}| \\ 0 \ 1 \end{pmatrix},$$

$$(27)$$

such that the reduced matrices \mathbf{M}^{\dagger} do not depend on possibly huge $|e^{\sigma_j|S_j|}|$.

Proof. The statement follows directly from Eqs. (26), (24), and (20).

Lemma 4. Matrices \mathbf{M}^{\dagger} translate Robin BCs

$$F'(0) = \sigma_L F(0), \qquad F'(Z) = -\sigma_U F(Z),$$
 (28)

of Eqs. (21) and (22) to similar conditions at any material layer interface z_j , j = 1, ..., m - 1:

$$F'(z_j) = \eta_{j+1}^L F(z_j), \qquad \eta_{j+1}^L = \frac{M_{[j,0],21}^{\dagger +}(\sigma) + \sigma_L M_{[j,0],22}^{\dagger +}(\sigma)}{\sigma_L M_{[j,0],12}^{\dagger +}(\sigma) + M_{[j,0],11}^{\dagger +}(\sigma)},$$

$$F'(z_j) = -\eta_j^U F(z_j), \qquad \eta_j^U = \frac{M_{[j,m],21}^{\dagger -}(\sigma) - \sigma_U M_{[j,m],22}^{\dagger -}(\sigma)}{\sigma_U M_{[j,m],12}^{\dagger -}(\sigma) - M_{[j,m],11}^{\dagger -}(\sigma)}.$$
(29)

Proof. Eqs. (29) can be easily derived by relating the vectors $\binom{F}{F'}(0)$ or $\binom{F}{F'}(Z)$ with $\binom{F}{F'}(z_j)$ using transfer matrices $\mathbf{M}(z_j, z_0; \sigma)$ or $\mathbf{M}(z_j, z_m; \sigma)$, see Eq. (26), exploring the reduced form of \mathbf{M} given in Eq. (27), and solving the resulting equations together with the BCs (28).

Algorithm 1. To avoid problems induced by computer arithmetics when working with almost vanishing numbers, for calculations of factors $\eta^{L,U}$, one should better use the recurrent expressions, which do not fail even when in some $S_i \Gamma_i \to 1$ and still are well defined when $|\sigma_i| \to 0$ and $\Gamma_i \to 0$:

$$\eta_{1}^{L} = \sigma_{L}, \quad \left[\eta_{j+1}^{L} - \sigma_{j}\right] = \frac{(\eta_{j}^{L} - \sigma_{j})(1 - \Gamma_{j})^{2}}{(1 + \Gamma_{j}^{2}) + \frac{2\Gamma_{j}}{\sigma_{j}}\eta_{j}^{L}} \xrightarrow{\sigma_{j} \to 0} \frac{\eta_{j}^{L}}{1 + |S_{j}|\eta_{j}^{L}}, \quad 1 \le j < m,$$

$$\eta_{m}^{U} = \sigma_{U}, \quad \left[\eta_{j-1}^{U} - \sigma_{j}\right] = \frac{(\eta_{j}^{U} - \sigma_{j})(1 - \Gamma_{j})^{2}}{(1 + \Gamma_{j}^{2}) + \frac{2\Gamma_{j}}{\sigma_{j}}\eta_{j}^{U}} \xrightarrow{\sigma_{j} \to 0} \frac{\eta_{j}^{U}}{1 + |S_{j}|\eta_{j}^{U}}, \quad m \ge j > 1.$$
(30)

These conditions can be derived by transferring the Robin-type relations of F and F' at material interfaces z_j by a single adjacent material layer to z_{j+1} (using the matrix $\mathbf{M}_{[j+1]}^{\dagger+}(\sigma_{j+1})$ from Eq. (27), obtaining the following η_{j+2}^L) or z_{j-1} (using $\mathbf{M}_{[j]}^{\dagger-}(\sigma_j)$, obtaining η_{j-1}^U). When $\Gamma_j \approx 1$, the expressions at both sides of the equations are also small, and we avoid undesired additions and subtractions of small and moderate numbers in this formula.

Remark 3. Algorithm 1 can also be used for Dirichlet BCs, F(0) = F(Z) = 0 ($\rho = 0$ in BCs (9), for example). The procedure (30) should be started from $\left[\eta_2^L - \sigma_1\right] = \frac{\sigma_1(1-\Gamma_1)^2}{2\Gamma_1}$ and $\left[\eta_{m-1}^U - \sigma_m\right] = \frac{\sigma_m(1-\Gamma_m)^2}{2\Gamma_m}$ in this case.

3.2 Vertical mode and its intensity

To identify the required vertical mode $\Theta(z)$ and effective refractive index n_{\bullet} , we substitute the onedimensional Helmholtz problem (7), (8), (9) with the root-finding of the related algebraic (characteristic) equation [4, 2] and the reconstruction of $\Theta(z)$ using transfer matrices \mathbf{M} afterward.

Theorem 1. The problem (7), (8), (9) with $\rho \in \{0, 1\}$ has a nontrivial solution $\Theta(z) \in C^2(\cup_{j=1}^m S_j) \cup C^1([0, Z])$ if and only if the characteristic equality

$$0 = \chi(\sigma) \stackrel{def}{=} \begin{cases} (\sigma_U \ 1) \mathbf{M}(Z, 0; \sigma) \begin{pmatrix} 1 \\ \sigma_L \end{pmatrix} & \text{if } \rho = 1 \quad [\text{Robin BC}] \\ M_{12}(Z, 0; \sigma) & \text{if } \rho = 0 \quad [\text{Dirichlet BC}] \end{cases}$$
(31)

holds. Here (2×2) -matrix $\mathbf{M}(Z, 0; \sigma)$ is constructed as suggested in Lemma 3.

Proof. Let $\Theta(z)$ be a nontrivial solution to the considered problem. Assume first that $\rho = 1$, such that $\Theta(0) \neq 0$. Otherwise, due to BCs (9), $\begin{pmatrix} \Theta \\ \Theta' \end{pmatrix}$ vanishes at z = 0, while Lemmas 3 and 2 imply the vanishing of $\Theta(z)$ at all layer interfaces and within all layers, respectively. The same consideration allows us to conclude that $\Theta(Z) \neq 0$ as well. Translation of the nontrivial $\begin{pmatrix} \Theta \\ \Theta' \end{pmatrix}(0)$ over [0, Z] using $\mathbf{M}(Z, 0; \sigma)$ and applying BCs (9) to eliminate $\Theta'(0)$ and $\Theta'(Z)$ from the resulting relation implies the condition $\begin{pmatrix} 1 \\ -\sigma_U \end{pmatrix} \Theta(Z) = \mathbf{M}(Z, 0; \sigma) \begin{pmatrix} 1 \\ \sigma_L \end{pmatrix} \Theta(0)$, which, after the multiplication of both sides by the row-vector ($\sigma_U 1$) from the left and accounting for the statements of Corollary 3, gives characteristic Eq. (31). Assume now that $\chi(\sigma) = 0$, i.e.,

$$-\sigma_U[M_{11}(Z,0;\sigma) + \sigma_L M_{12}(Z,0;\sigma)] = M_{21}(Z,0;\sigma) + \sigma_L M_{22}(Z,0;\sigma).$$

Let us translate a vector $\binom{1}{\sigma_L}$ (satisfying BCs (9) at z = 0) with $\mathbf{M}(z, 0; \sigma)$ over [0, Z], obtaining nontrivial $\Theta(z)$ and $\Theta'(z)$ in this way. Within [0, Z], $\Theta(z)$ solves Eqs. (7), (8). At z = Z, $\binom{\Theta}{\Theta'}(Z) = \mathbf{M}(Z, 0; \sigma)\binom{1}{\sigma_L} \propto \binom{1}{-\sigma_U}$, i.e., $\Theta(z)$ satisfies BCs (9) at z = Z and, thus, solves our problem.

For $\rho = 0$, the BCs (9) are of Dirichlet-type, such that a nontrivial $\Theta(z)$ should have non-vanishing $\Theta'(0)$ and $\Theta'(Z)$. Translation of $\begin{pmatrix} 0 \\ \Theta'(0) \end{pmatrix}$ over [0, Z] implies $\begin{pmatrix} 0 \\ 1 \end{pmatrix} \Theta'(Z) = \mathbf{M}(Z, 0; \sigma) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Theta'(0)$, which gives us $\chi(\sigma) = 0$ in (31). On the other hand, if $\chi(\sigma) = 0$, by propagating $\begin{pmatrix} \Theta \\ \Theta' \end{pmatrix}(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ over [0, Z], we obtain a nontrivial $\Theta(z)$ solving Eqs. (7), (8), and at z = Z satisfying the relation $\Theta(Z) = \chi(\sigma)$, i.e., fulfilling Dirichlet BCs in (9).

Corollary 4. Matrix $\mathbf{M}(Z, 0; \sigma)$ in Eq. (31) can be replaced by $\mathbf{M}_{[m,0]}^{\dagger+}(\sigma)$ or by another matrix $\mathbf{M}_{[m,0]}^{\dagger\dagger+}(\sigma)$ obtained after substituting $\mathbf{M}_{[j]}^{\dagger+}(\sigma_j)$ within some layers S_j in Eq. (27) with the original layer-wise propagator $\mathbf{M}_j(z_j, z_{j-1}; \sigma_j)$.

Proof. The proof is identical to that of Theorem 1, since these matrices can be obtained from $\mathbf{M}(Z, 0; \sigma)$ by multiplying it with a non-vanishing factor composed of all or several multipliers $e^{-\sigma_j |S_j|}$.

Theorem 1 and Corollary 4 define the characteristic equation $\chi(n_{\bullet}) \stackrel{def}{=} \chi(\tilde{\sigma}(n_{\bullet}, n(z))) = 0. \tilde{\sigma}$ is defined in Eq. (7), and n(z) is a layer-wise constant positive real function introduced at the beginning

of Section 3. Since n(z) is real, all physically relevant n_{\bullet} satisfying Eq. (8) and, thus, Eq. (31) are also real and belong to the interval $(0, \max_z n(z)]$. To find these roots, we scan $\chi(\xi)$ along the suggested interval, detect rough approximations of n_{\bullet} on the way, and correct them using the Newton-Raphson iterative procedure, exploring analytic expressions for χ and χ' given by the following algorithm:

Algorithm 2. Assume that the characteristic function (31) is constructed using the matrix $\mathbf{M}_{[m,0]}^{\dagger+}(\sigma)$ (27), where a layer-wise constant $\sigma(z)$ defining parameters $\sigma_{L,U} \neq 0$ and σ_r , $r = 1, \ldots, m$, are functions of the variable ξ (7). Accounting that $\frac{d}{d\xi}\sigma_{\nu}(\xi) = \frac{k_0^2\xi}{\sigma_{\nu}(\xi)}$, we can construct $\chi(\tilde{\sigma}(\xi, n(z))) = \chi(\xi)$ and its ξ -derivative using the recurrent matrix-vector multiplication procedure:

$$\chi(\xi) = {\binom{\sigma_U}{1}}^T \mathcal{F}_m(\xi), \ \chi'(\xi) = {\binom{\sigma_U}{1}}^T \mathcal{F}'_m(\xi) + \frac{k_0^2 \xi}{\sigma_U} {\binom{1}{0}}^T \mathcal{F}_m(\xi), \ \text{where}$$

$$\begin{cases}
\mathcal{F}_r(\xi) \stackrel{def}{=} \mathbf{M}_{[r]}^{\dagger +}(\sigma_r) \mathcal{F}_{r-1}(\xi) \\
\mathcal{F}'_r(\xi) \stackrel{def}{=} \mathbf{M}_{[r]}^{\dagger +}(\sigma_r) \mathcal{F}'_{r-1}(\zeta) + \frac{k_0^2 \xi \frac{d}{d\sigma} \mathbf{M}_{[r]}^{\dagger +}(\sigma_r)}{\sigma_r} \mathcal{F}_{r-1}(\xi), \ 1 \le r \le m; \\
\mathcal{F}_0(\xi) = {\binom{1}{\sigma_L}}, \ \mathcal{F}'_0(\xi) = \left[\frac{d}{d\sigma_L} {\binom{1}{\sigma_L}}\right] \frac{d\sigma_L}{d\xi} = \frac{k_0^2 \xi}{\sigma_L} {\binom{0}{1}}.
\end{cases}$$
(32)

If $\sigma_j(\xi) \to 0$, factor $\mathcal{F}'_j(\xi)$ is undefined. Thus, following the statement of Corollary 4, for those layers where $|e^{|S_j|\sigma_j(\xi)}|$ remains moderate (1 for $\sigma_j = 0$), during the construction of $\chi(\xi)$ instead of $\mathbf{M}^{\dagger+}_{[j]}(\sigma_j)$, one should better use $\mathbf{M}_j(z_j, z_{j-1}; \sigma_j)$, which has a well-defined ξ -derivative even for vanishing σ_j :

$$\frac{d}{d\xi}\mathbf{M}_j(z_j, z_{j-1}; \sigma_j(\xi)) = \frac{k_0^2 \xi \frac{d}{d\sigma} \mathbf{M}_j(z_j, z_{j-1}; \sigma_j)}{\sigma_j} \xrightarrow{\sigma_j \to 0} k_0^2 \xi |S_j| \begin{pmatrix} |S_j| & \frac{|S_j|^2}{3} \\ 2 & |S_j| \end{pmatrix}.$$

Algorithm 3. After finding vertical-mode-defining n_{\bullet} , we reconstruct the vertical mode and find its layer-wise intensities \mathcal{P}_i^{Θ} using the following steps:

- i) Find $\sigma_j = \tilde{\sigma}(n_{\bullet}, n_j)$, $1 \le j \le m$ (and $j \in \{L, U\}$, if $\rho = 1$ in Eq. (9));
- ii) Find factors η^L (or η^U) for Robin-type relations of Θ and Θ' (29) at the border z_k of the active zone or PC layer (where |Θ| is expected to be large) using Algorithm 1 (and Remark 3, if Dirichlet BCs are considered);
- iii) Set $\binom{\Theta_u}{\Theta'_u}(z_k) = \binom{1}{\eta_{k+1}^L}$ and propagate this vector towards z = Z and z = 0 with transfer matrices (26) and (24). The selection of z_k allows us to avoid large exponential growth within the layers S_j with large $\Re \sigma_j |S_j|$. Here, we can have less vital exponential decay towards zero instead;
- iv) During propagation, collect $\Theta_u(z)$ at the layer borders and use them to evaluate the mode power $\mathcal{P}_j^{\Theta_u}$ in each layer S_j ; see Eqs. (12) and (25) for the definition of matrix \mathbf{p}_j . For Robin BCs, we have $\Theta_u(\pm \infty) = 0$ and $\Gamma_{0,m+1} \to 1$, s. t. in the infinitely long outside regions S_0 and S_{m+1} the relations $\mathcal{P}_0^{\Theta_u} = |\Theta_u(0)|^2/(2\sigma_L)$ and $\mathcal{P}_{m+1}^{\Theta_u} = |\Theta_u(Z)|^2/(2\sigma_U)$ hold;
- v) $\mathcal{P}_T^{\Theta_u} = \sum_{j=0}^{m+1} \mathcal{P}_j^{\Theta_u}$ is the overall intensity of the unscaled mode $\Theta_u(z)$. It is used for the final mode scaling, $\Theta(z) = \Theta_u(z)/(\mathcal{P}_T^{\Theta_u})^{1/2}$, and for defining the scaled mode power within the layers, $\mathcal{P}_j^{\Theta} = \mathcal{P}_j^{\Theta_u}/\mathcal{P}_T^{\Theta_u}$.

An example with six calculated vertical modes (lines) and corresponding function n(z) (red dots) is shown in Fig. 2. We used vertical structure and PC cell size a from Ref. [6] and Robin BCs with





Figure 2: Six calculated scaled vertical modes (solid lines) and corresponding function n(z) (red dots). Magenta: the main mode used for construction of C.

Figure 3: Green's functions $G_{(0,0)}$ (magenta), $G_{(1,1)}$ (green), and $G_{(2,2)}$ (light blue) at fixed z' within the PC layer. Solid and dashed: real and imaginary parts of G_p .

 $n_{L,U} = 1$ in calculations. Since the description of the PC layer was not complete, we used unit cells containing a pair of by air-filled 45° slanted ellipses centered at $(x_{\pm}, y_{\pm}) = (\pm \frac{a}{8}, \pm \frac{a}{8})$, see the middle diagram of Fig. 1(d), allowing to have in Ref. [6] reported effective refractive index $n_{\bullet} \approx 3.429$. Besides the broad n- and p-cladding layers at the edges of the figure, we distinguish an active region composed of three quantum wells (QWs) and a PC layer. The mode with the largest n_{\bullet} and largest intensity within the QW layer is the vertical mode of our interest.

3.3 Green's function and related integral expressions

Below, we build matrices $\mathbf{g}_p^{(k,j)}$ (12), which, together with the values of Θ at the PC layer edges, enable finding integrals $\mathcal{G}_p^{(k,j)}$ used to construct matrix **C**. When reconstructing $G_p(z, z')$ [8] for $(z, z') \in S_k \times S_j$, we distinguish the cases of k = j and $k \neq j$. In the first case, for $z \in \bigcup_{l=1}^{j-1} S_l$ and $z \in \bigcup_{l=j+1}^m S_l$, and z' considered as a parameter, Green's function defining Eqs. (13), (14) are similar to (21), (28). We use matrices \mathbf{M}^{\dagger} and Algorithm 1 to calculate factors $\eta_{p,j}^L$ and $\eta_{p,j}^U$, determining Robin BCs (29) at the edges of S_j . In both subregions z < z' and z > z' of the square $S_j \times S_j$, the Green's functions are solutions of the homogeneous Eq. (13), i.e., they can be written as³

$$G_p(z,z') = \begin{cases} B_{p,j}^{L+}(z')e^{\sigma_{p,j}z} + B_{p,j}^{L-}(z')e^{-\sigma_{p,j}z} & \text{for } z < z' \\ B_{p,j}^{U+}(z')e^{\sigma_{p,j}z} + B_{p,j}^{U-}(z')e^{-\sigma_{p,j}z} & \text{for } z > z' \end{cases}.$$
(33)

 $G_p(z, z')$ satisfies BCs (29) at $z = z_{j-1}$ and z_j and the connection conditions (16) at z = z'. By resolving the resulting system of four inhomogeneous equations w.r.t. four variables $B_{p,j}^{L\pm}$, $B_{p,j}^{U\pm}$, we

³Note that $|p| \neq 1$, such that $|\sigma_{p,j}|$ is not vanishing.

can rewrite $G_p(z, z')$ as

$$G_{p}(z, z') = \frac{e^{-\sigma_{p,j}|z-z'|}}{2\sigma_{p,j}} + \mathcal{E}_{p,j}^{T}(z')\mathbf{B}_{p,j}\mathcal{E}_{p,j}(z), \text{ where}$$

$$\mathcal{E}_{p,j}(\xi) = (1 + \Gamma_{p,j}) \begin{pmatrix} e^{\sigma_{p,j}(\xi-z_{j})} \\ e^{\sigma_{p,j}(z_{j-1}-\xi)} \end{pmatrix}, \\
\mathbf{B}_{p,j} = \begin{pmatrix} \frac{(\sigma_{p,j} + \eta_{p,j}^{L})(\sigma_{p,j} - \eta_{p,j}^{U})}{2\sigma_{p,j}\Delta_{p,j}} & \frac{(\sigma_{p,j} - \eta_{p,j}^{L})(\sigma_{p,j} - \eta_{p,j}^{U})(1 - \Gamma_{p,j})}{2\sigma_{p,j}\Delta_{p,j}(1 + \Gamma_{p,j})} \\ \frac{(\sigma_{p,j} - \eta_{p,j}^{L})(\sigma_{p,j} - \eta_{p,j}^{U})(1 - \Gamma_{p,j})}{2\sigma_{p,j}\Delta_{p,j}(1 + \Gamma_{p,j})} & \frac{(\sigma_{p,j} - \eta_{p,j}^{L})(\sigma_{p,j} + \eta_{p,j}^{U})}{2\sigma_{p,j}\Delta_{p,j}} \end{pmatrix}, \\
\Delta_{p,j} = (\sigma_{p,j} + \eta_{p,j}^{L})(\sigma_{p,j} + \eta_{p,j}^{U})(1 + \Gamma_{p,j})^{2} \\ -(\sigma_{p,j} - \eta_{p,j}^{L})(\sigma_{p,j} - \eta_{p,j}^{U})(1 - \Gamma_{p,j})^{2}. \end{cases}$$
(34)

Inspired by the form of $G_p(z, z')$ within $S_j \times S_j$, given as a linear combination of four exponentials $e^{\nu\sigma_{p,j}z}e^{\nu'\sigma_{p,j}z'}$, $\{\nu, \nu'\} \in \{\pm\}$, we seek to write G_p for any $z' \in S_j$ and z belonging to any of material interfaces, $z = z_l$, 0 < l < m, as

$$G_p(z_l, z') = \mathcal{J}_{p,l}^{jT} \mathcal{E}_{p,j}(z'), \quad \text{with } z' \text{-independent } \mathcal{J}_{p,l}^j = \begin{pmatrix} \mathcal{J}_{p,l}^{j+} \\ \mathcal{J}_{p,l}^{j-} \end{pmatrix}.$$
(35)

Indeed, at both sides of the S_i -layer, Eq. (34) provides the relations

$$\mathcal{J}_{p,j-1}^{j\pm} = \frac{(1 \pm \Gamma_{p,j})(\sigma_{p,j} \pm \eta_{p,j}^U)}{\Delta_{p,j}}, \quad \mathcal{J}_{p,j}^{j\pm} = \frac{(1 \pm \Gamma_{p,j})(\sigma_{p,j} \pm \eta_{p,j}^L)}{\Delta_{p,j}}.$$
 (36)

Since $z' \in S_j$, Green's function defining Eq. (13) is homogeneous for $z \leq z_{j-1}$ and $z \geq z_j$. Due to Lemma 3 and Corollary 3, one can translate $\binom{G_p}{\partial_z G_p}(z, z')$ from z_{j-1} to z_l , l < j - 1, and z_j to z_l , l > j, using matrices $\mathbf{M}_{[l]}^{\dagger-}(\sigma_{p,l})$ and $\mathbf{M}_{[l]}^{\dagger+}(\sigma_{p,l})$ (27), respectively. Exploiting the relations $\partial_z G_p(z_l, z') = \eta_{p,l+1}^L G_p(z_l, z')$, l < j, and $\partial_z G_p(z_l, z') = -\eta_{p,l}^U G_p(z_l, z')$, $l \geq j$, with factors $\eta^{L,U}$ derived following Algorithm 1 and collecting the terms at the corresponding exponentials $e^{\pm \sigma_{p,l}(z'-\bar{z}_l)}$ provide the required relations

$$\mathcal{J}_{p,l-1}^{j\pm} = \frac{\sigma_{p,l}(1-\Gamma_{p,l}^{2})}{\sigma_{p,l}(1+\Gamma_{p,l}^{2})+2\eta_{p,l}^{L}\Gamma_{p,l}} \mathcal{J}_{p,l}^{j\pm}, \quad l = j-1, \dots, 1, \\
\mathcal{J}_{p,l}^{j\pm} = \frac{\sigma_{p,l}(1-\Gamma_{p,l}^{2})}{\sigma_{p,l}(1+\Gamma_{p,l}^{2})+2\eta_{p,l}^{U}\Gamma_{p,l}} \mathcal{J}_{p,l-1}^{j\pm}, \quad l = j+1, \dots, m.$$
(37)

For any $k \neq j$ and $z \in S_k$, parametrically on $z' \in S_j$ depending $G_p(z, z')$ satisfies homogeneous Eq. (21) and, thus, is defined by the analog of Eq. (23) with boundary values $\mathcal{B}_k^{G_p(\cdot,z')}$ (i.e., $G_p(z_{k-1}, z')$ and $G_p(z_k, z')$) given by Eqs. (35), (36), (37) and $\theta_{p,k}(z)$ defined using $\sigma_{p,k}$ instead of σ_k . One can show that in each subregion $S_k \times S_j$, $k \neq j$, $G_p(z, z')$ can be written as

$$G_{p}(z, z') = \mathcal{E}_{p,j}^{T}(z') \mathbf{A}_{p,k}^{j} \mathcal{E}_{p,k}(z), \quad \text{where} \\ \mathbf{A}_{p,k}^{j} = \begin{cases} A_{p,k}^{\dagger j} \mathcal{J}_{p,k}^{j} \binom{(1+\Gamma_{p,k})(\sigma_{p,k}+\eta_{p,k}^{L})}{(1-\Gamma_{p,k})(\sigma_{p,k}-\eta_{p,k}^{L})} \end{bmatrix}^{T} & \text{if } k < j \\ A_{p,k}^{\dagger j} \mathcal{J}_{p,k-1}^{j} \binom{(1-\Gamma_{p,k})(\sigma_{p,k}-\eta_{p,k}^{U})}{(1+\Gamma_{p,k})(\sigma_{p,k}+\eta_{p,k}^{U})} \end{bmatrix}^{T} & \text{if } k > j \end{cases}$$

$$A_{p,k}^{\dagger j} = \frac{1}{2(1+\Gamma_{p,k}^{2})\sigma_{p,k}+2\Gamma_{p,k}\left[(\eta_{p,k}^{L}+\eta_{p,k}^{U})-\operatorname{sgn}(k-j)(\eta_{p,k}^{L}-\eta_{p,k}^{U})\right]}.$$
(38)

Examples of three Green's functions $G_p(z, z')$ for p = (0, 0), (1, 1), and (2, 2) for the fixed z' and the parameters explored in Fig. 2 are shown in Fig. 3. For |p| = 0, the function has non-vanishing and,

within each but z'-containing layer, harmonically oscillating real and imaginary parts. For the remaining p, $\Im G_p$ vanishes, and the function is represented by a sharp exponentially growing/decaying spike at z = z'. This shape of G_p suggests that for large |p|, a proper fully numerical estimation of the integral expressions \mathcal{G}_p can require a very fine numerical mesh and, thus, a considerable computational time.

Let us switch to calculating matrices $\mathbf{g}_p^{(k,j)}$ from Eq. (12). For contributions due to continuously differentiable part of G_p (defined by matrices **B** and **A** in Eqs. (34), (38)), separation of variables z and z' is possible, and we only need to calculate layer-wise integrals of the matrix-function $\theta_j(z)\mathcal{E}_{p,j}^T(z)$. $\mathcal{E}_{p,j}$ and θ_j are by exponents and by combinations of exponents defined vector-functions, see Eqs. (34) and (23), respectively.

$$\mathbf{I}_{p,j} = \begin{pmatrix} I_{p,j}^+ & I_{p,j}^- \\ I_{p,j}^- & I_{p,j}^+ \end{pmatrix} \stackrel{def}{=} \int_{S_j} \theta_j(z) \mathcal{E}_{p,j}^T(z) dz, \quad \text{where} \\ I_{p,j}^{\pm} = \frac{(\sigma_{p,j} \mp \sigma_j \Gamma_j)(\Gamma_{p,j} \pm 1) \mp \frac{\sigma_j}{\Gamma_j}(1 - \Gamma_j^2) \Gamma_{p,j}}{(\sigma_{p,j}^2 - \sigma_j^2)} \xrightarrow{\sigma_j \to 0} \frac{\sigma_{p,j} |S_j|(\Gamma_{p,j} \pm 1) \mp 2\Gamma_{p,j}}{\sigma_{p,j}^2 |S_j|}.$$
(39)

The least trivial is the major contribution to $\mathbf{g}_p^{(j,j)}$, which involves double-integration of $e^{-\sigma_j|z-z'|}$ over $S_j \times S_j$ and requires splitting the inner integration region into two subintervals $[z_{j-1}, z]$ and $[z, z_j]$. Still, we can show that

$$\int_{S_{j}S_{j}} \theta_{j}(z') \frac{e^{-\sigma_{p,j}|z-z'|}}{2\sigma_{p,j}} dz' \theta_{j}^{T}(z) dz = \frac{\mathbf{p}_{j}}{(\sigma_{p,j}^{2} - \sigma_{j}^{2})} - \mathbf{I}_{p,j} \mathbf{R}_{p,j} \mathbf{I}_{p,j}, \text{ where}
\mathbf{R}_{p,j} = R_{p,j}^{\dagger} \begin{pmatrix} R_{p,j}' & R_{p,j}'' \\ R_{p,j}'' & R_{p,j}' \end{pmatrix}, \qquad R_{p,j}' = \frac{(\sigma_{p,j}^{2} - \sigma_{j}^{2})}{\sigma_{p,j}(1 + \Gamma_{j})} \xrightarrow{\sigma_{j} \to 0} \sigma_{p,j},
R_{p,j}'' = \frac{(\sigma_{p,j}^{2} + \sigma_{j}^{2})(1 - \Gamma_{p,j}) + 2\frac{\sigma_{j}}{\Gamma_{j}} \sigma_{p,j}(\Gamma_{j}^{2} - \Gamma_{p,j})}{\sigma_{p,j}(1 + \Gamma_{j})(1 + \Gamma_{p,j})} \xrightarrow{\sigma_{j} \to 0} \frac{(1 - \Gamma_{p,j})\sigma_{p,j}|S_{j}| - 4\Gamma_{p,j}}{(1 + \Gamma_{p,j})|S_{j}|},
R_{p,j}^{\dagger} = \frac{(1 + \Gamma_{j})}{8\left(\sigma_{p,j} - \frac{\sigma_{j}}{\Gamma_{j}}\Gamma_{p,j}\right)\left(\sigma_{p,j}\Gamma_{p,j} - \sigma_{j}\Gamma_{j}\right)} \xrightarrow{\sigma_{j} \to 0} \frac{|S_{j}|}{8\Gamma_{p,j}\sigma_{p,j}(\sigma_{p,j}|S_{j}| - 2\Gamma_{p,j})}.$$
(40)

The expressions for $\mathbf{g}_p^{(k,j)}$ now can be written as

$$\mathbf{g}_{p}^{(k,j)} = \begin{cases} \frac{\mathbf{p}_{j}}{(\sigma_{p,j}^{2} - \sigma_{j}^{2})} + \mathbf{I}_{p,j} [\mathbf{B}_{p,j} - \mathbf{R}_{p,j}] \mathbf{I}_{p,j} & \text{if } k = j \\ \mathbf{I}_{p,j} \mathbf{A}_{p,k}^{j} \mathbf{I}_{p,k} & \text{if } k \neq j \end{cases}.$$
(41)

Recall that $\sigma_{p,j}$ is non-vanishing, $\sigma_{p,j}$ and $\eta_{p,j}^{L,U}$ can be similar (corresponding differences are small), and, especially for large |p|, factor $\Gamma_{p,l} \approx 1$, which should be ever accounted for when estimating the required expressions.

All formulas in this Subsection are written avoiding summations of numbers differing by many orders and divisions of very small or very large numbers. Such arithmetic operations, used in sometimes more compact formulas for \mathcal{P}_{j}^{Θ} and $\mathcal{G}_{(r,s)}^{(k,j)}$, have led to inaccuracies of computer arithmetics and violations of calculations in our first version of the numerical code.

3.4 Truncation of the coupling matrix

As it was indicated in Eq. (17), C, or, more precisely, C_{2D} , relies on the infinite sum of submatrices $C_{2D}^{(r,s)}$, depending on the Fourier coefficients $\xi_{r\pm 1,s}^{j}$, $\xi_{r,s\pm 1}^{j}$ (11) of the squared refractive index, vertical mode intensities \mathcal{P}_{j}^{Θ} within PC sublayers S_{j} , and integral factors $\mathcal{G}_{(r,s)}^{(k,j)}$ with integration performed in the PC sublayer-defined regions $S_{k} \times S_{j}$. By the finite (truncated) sum

$$\mathbf{C}_{2D}^{(M)} = \sum_{|r|+|s|>1, \{|r|, |s|\} \le M} \mathbf{C}_{2D}^{(r,s)},\tag{42}$$

we denote approximations of C_{2D} obtained using the truncation parameter M. The Fourier coefficients $\xi_{r,s}^j$ are obtained using the Fast Fourier Transform (FFT) of the uniformly in the unit cell of the PC discretized function $\bar{n}^2(x, y, z)|_{z \in S_j}$. Thus, calculations of $C_{2D}^{(M)}$ are only possible if the number of discretization steps along the cell sides more than twice exceeds the parameter M. In the calculation examples of Fig. 4, we used the model parameters as in Figs. 2 and 3 and a uniform $2^{11} \times 2^{11}$ discretization of the unit cell, which is sufficient for construction of the truncated sums with up to M = 1022.



Figure 4: Calculations of $\mathbf{C}_{2D}^{(M)}$ in dependence on the truncation parameter M (42). (a): Time required for calculations of $\mathbf{C}_{2D}^{(M)}$ in the same PCSEL with 1, 3, and 5 PC layers. (b): Relative error of $\mathbf{C}_{2D}^{(M)}$ elements as function of M. Inset: moduli of these elements. (c): spectrum of $i\mathbf{C}$ in dependence on M. X: eigenvalues of $i\mathbf{C}$ obtained using $\mathbf{C}_{2D}^{(20)}$.

In Fig. 4(a), we show the time needed for calculations of $\mathbf{C}_{2D}^{(M)}$ with different M when the PCSEL has a single PC layer (magenta) or this layer is subdivided into three (green) and five (light blue) sublayers, respectively. With an increase of M, this time grows quadratically in all three cases, which is in accord with a quadratic growth of the parameter set $\{(r,s)\}$ satisfying the summation conditions in Eq. (42). An increase in the number of PC sublayers implies another, approximately quadratic, growth of the calculation time, which is due to the necessity of estimating factors $\mathcal{G}_p^{(k,j)}$ for growing sets of PC layer indices $\{(k,j)\}$ (recall that in the structure with a single PC layer S_k , a single factor $\mathcal{G}_p^{(k,k)}$ is needed for each value of |p|). We note that Fig. 4(a) shows only the time needed for the estimation of $\mathbf{C}_{2D}^{(M)}$. Time spent for construction of the whole matrix \mathbf{C} using M = 1020 (including reading and preprocessing of model parameters, 2-dimensional FFT of $\bar{n}(x, y, z)$, and finding the vertical mode and the remaining components of \mathbf{C}) was about 41, 107, and 268 s in 1-, 3-, and 5-PC-layer cases, respectively. In contrast to the above-used analytic formulas, calculations of $\mathbf{C}_{y}^{(k,j)}$ took the whole day and even more.

Fig. 4(b) shows the evolution of the relative error $|(\mathbf{C}_{2D,ij}^{(M)} - \mathbf{C}_{2D,ij})/\mathbf{C}_{2D,ij}|$ (main diagram, $\mathbf{C}_{2D}^{(1020)}$ was used instead of the exact \mathbf{C}_{2D}) and $|\mathbf{C}_{2D,ij}^{(M)}|$ (insert) with an increase of M. Since \mathbf{C}_{2D} is Hermitian [6, 7] and due to the symmetry of the PC unit cell w.r.t. y = x line, the moduli of all 16 components of \mathbf{C}_{2D} are represented by these four curves. One can see that M = 160 is sufficient to reduce the relative errors of the matrix \mathbf{C}_{2D} elements to 1% and less in this case. In practical calculations, where estimation of the eigenvalues (especially their real parts) of the spectral problem (3) is required, even smaller values of M can also be sufficient. The illustration is given in Fig. 4(c), showing changes in the spectra of $i\mathbf{C}$ calculated using truncated $\mathbf{C}_{2D}^{(M)}$ with an increase of M. Crosses in this diagram, representing the eigenvalues $\Lambda_{i\mathbf{C}}$ obtained with a moderate value of M = 20, have nearly the same

real parts and not so much distinguishable imaginary parts as the eigenvalues calculated using high M (indicated by dark bullets in the same figure). Since Λ_{iC} give us decent approximations of the exact eigenvalues solving the spectral problem (3) in the case of $L \to \infty$, we expect that moderate M values can be sufficient when considering the spectral problem for large but still finite L.

4 Numerical solution of the spectral problem

Similar spectral problems defined for domains with one spatial variable occur, e.g., in the analysis of edge-emitting distributed-feedback lasers. Often, these problems can be solved exactly for a finite number of modes using transfer matrices, corresponding characteristic functions, and replacement of the spectral problem by the root-finding problem [9], as it was done in Theorem 1 and Subsection 3.2. In the limit case of fully decoupled cross-propagating field functions Φ_u and Φ_v , i.e., when off-diagonal 2×2 blocks of matrix C are 0, problem (3) splits into a pair of similar effectively one-dimensional problems. As will be shown later in this work, exact eigenvalues Λ_{1D} for this limit-case problem can still provide reasonable approximations for certain eigenvalues of the whole system. In this work, we use a fully numerical approach based on finite difference approximations to find the modes in the general case.

To construct a numerical scheme for the spectral problem (3), we subdivide the domain $(x, y) \in [0, L] \times [0, L]$ into n^2 squares with the side length $h = \frac{L}{n}$, and introduce the staggered mesh,

$$\omega_{u}^{h} = \omega_{x}^{\prime h} \times \omega_{y}^{\prime \prime h} \quad \text{and} \quad \omega_{v}^{h} = \omega_{x}^{\prime \prime h} \times \omega_{y}^{\prime h}, \quad \text{where}
\omega_{\xi}^{\prime h} = \{\xi_{j} = jh, \ 0 \le j \le n\}, \quad \omega_{\xi}^{\prime \prime h} = \{\xi_{j-\frac{1}{2}} = (j-\frac{1}{2})h, \ 1 \le j \le n\},$$
(43)

represented with black and red bullets in Fig. 5. This mesh defines the grid function Φ^h with 4n(n+1) components:

$$\Phi^{h} = \begin{pmatrix} \Phi^{h}_{u} \\ \Phi^{h}_{v} \end{pmatrix}, \quad \Phi^{h}_{u} = \begin{pmatrix} \Phi^{h+}_{u} \\ \Phi^{h-}_{u} \end{pmatrix}, \quad \Phi^{h}_{v} = \begin{pmatrix} \Phi^{h+}_{v} \\ \Phi^{h-}_{v} \end{pmatrix}, \quad \text{where}$$

$$\Phi^{h\pm}_{u,j,l-0.5} \approx \Phi^{\pm}_{u}(x_{j}, y_{l-0.5}), \quad \Phi^{h\pm}_{v,j-0.5,l} \approx \Phi^{\pm}_{v}(x_{j-0.5}, y_{l}). \tag{44}$$

These components are variables of the linear system consisting of $4n^2$ equations approximating each of four equations in (3) at n^2 spatial positions $\omega_x''^h \times \omega_y''^h$ (central positions of small squares in Fig. 5) and 4n BC-induced relations:

$$\begin{pmatrix} \sigma \partial_x^h & \mathbf{0} \\ \mathbf{0} & \sigma \partial_y^h \end{pmatrix} \Phi^h = \begin{bmatrix} i \mathbf{C} - \Lambda_h \end{bmatrix} \bar{\Phi}^h, \quad (x, y) \in \omega_x^{\prime\prime h} \times \omega_y^{\prime\prime h},$$

$$\Phi_{u,0,k-0.5}^{h+} = \Phi_{u,n,k-0.5}^{h-} = \Phi_{v,k-0.5,0}^{h+} = \Phi_{v,k-0.5,n}^{h-} = 0, \quad 1 \le k \le n.$$

$$(45)$$

Here, $\partial_x^h \Phi^h$, $\partial_y^h \Phi^h$, and $\overline{\Phi}^h$ are linear operators of the grid function Φ^h , providing finite-difference approximations of $\frac{\partial}{\partial x} \Phi$, $\frac{\partial}{\partial y} \Phi$, and Φ at $\omega_x''^h \times \omega_y''^h$.

4.1 Second order finite difference scheme

A simple approximation of Eqs. (3) at $\omega_x''^h \times \omega_y''^h$ is given by the second-order finite difference scheme (45), obtained using

$$\bar{\Phi}_{u,j,l}^{h\pm} \stackrel{def}{=} \sigma_j^h \Phi_{u,\cdot,l-0.5}^{h\pm}, \qquad \bar{\Phi}_{v,j,l}^{h\pm} \stackrel{def}{=} \sigma_l^h \Phi_{v,j-0.5,\cdot}^{h\pm},
\partial_x^h \Phi_{u,j,l}^{h\pm} \stackrel{def}{=} \sigma_j^{\dagger h} \Phi_{u,\cdot,l-0.5}^{h\pm}, \qquad \partial_y^h \Phi_{v,j,l}^{\pm} \stackrel{def}{=} \sigma_l^{\dagger h} \Phi_{v,j-0.5,\cdot}^{h\pm},$$
(46)



Figure 5: Scheme of the discretized computation domain. Bullets indicate spatial positions where mesh functions Φ_u^h and Φ_v^h are defined.



Figure 6: Schematics of sparse matrices H_h (nonvanishing black and red elements) and D_h (nonvanishing red elements) for the second order finite difference scheme.

where operators σ_k^h and $\sigma_k^{\dagger h}$ are given by

$$\sigma_k^h V^h = \frac{V_k^h + V_{k-1}^h}{2}, \qquad \sigma_k^{\dagger h} = \frac{V_k^h - V_{k-1}^h}{h}, \qquad 1 \le k \le n.$$
(47)

A discrete analog of conservation law (4) holds for Eqs. (45), (46), (47), which indicates good quality of the numerical scheme.

Lemma 5. Let Λ_h and nontrivial Φ^h satisfy Eqs. (45), (46), (47). Then

$$\mathcal{I}_{g}^{h} = \mathcal{I}_{v}^{h} + \mathcal{I}_{l}^{h}, \quad \text{where} \quad \mathcal{I}_{g}^{h} = -2\Re\Lambda_{h} \|\bar{\Phi}^{h}\|_{h}^{2}, \ \mathcal{I}_{v}^{h} = 2\Im(\bar{\Phi}^{h}, \mathbf{C}_{\mathrm{rd}}\bar{\Phi}^{h})_{h},$$
$$\mathcal{I}_{l}^{h} = h\sum_{j=1}^{n} |\Phi_{u,n,j-0.5}^{h+}|^{2} + |\Phi_{u,0,j-0.5}^{h-}|^{2} + |\Phi_{v,j-0.5,n}^{h+}|^{2} + |\Phi_{v,j-0.5,0}^{h-}|^{2}.$$
(48)

Here $\bar{\Phi}^h$ and $\mathbf{C}\bar{\Phi}^h$ are n^2 -component sets of four-component vectors $\bar{\Phi}^h_{j,l}$ and $\mathbf{C}\bar{\Phi}^h_{j,l}$; $(\bar{\xi}^h, \bar{\zeta}^h)_h = h^2 \sum_{j,l=1}^n \bar{\xi}^{h*T}_{j,l} \bar{\zeta}^h_{j,l}$ and $\|\bar{\xi}^h\|_h = (\bar{\xi}^h, \bar{\xi}^h)_h^{1/2}$ are discrete analogs of scalar products and norms introduced in Lemma 1.

Proof. Linear equations in (45) can be interpreted as a n^2 -component set of four-equation subsystems, each approximating Eq. (3) at different positions of $\omega_x''^h \times \omega_y''^h$. By applying the discrete scalar product with respect to this set and $2\bar{\Phi}^h$, taking the real part, and eliminating 4n boundary elements, we get $\mathcal{I}_l^h = 2\Re(\bar{\Phi}^h, i\mathbf{C}\bar{\Phi}^h)_h + \mathcal{I}_g^h$. As in Remark 1, the relation $2\Re(\bar{\Phi}^h, i\mathbf{C}\bar{\Phi}^h)_h = i(\bar{\Phi}^h, [\mathbf{C} - \mathbf{C}^{*T}]\bar{\Phi}^h)_h = \mathcal{I}_v^h$ immediately leads to the proof of this Lemma.

Substituting the expressions (46), (47) into Eq. (45), multiplying them by 2, and eliminating the BCs alow rewriting our schemes as a standard generalized spectral problem (or corresponding classical spectral problem):

$$\mathbf{H}_{h}W^{h} = \Lambda_{h}\mathbf{D}_{h}W^{h} \qquad \Leftrightarrow \qquad \mathbf{D}_{h}^{-1}\mathbf{H}_{h}W^{h} = \Lambda_{h}W^{h}.$$
(49)

Here, $4n^2$ -dimensional vector W^h contains all variables of Φ^h except for boundary elements from Eq. (45). \mathbf{H}_h and \mathbf{D}_h are sparse $4n^2 \times 4n^2$ -matrices with $\sim 32n^2$ and $\sim 8n^2$ non-vanishing elements

each. For example, we can set

$$W_{2j-1+2n(l-1)}^{h} = \Phi_{u,j-1,l-0.5}^{h-}, \qquad W_{2j+2n(l-1)}^{h} = \Phi_{u,j,l-0.5}^{h+}, W_{2l-1+2n(j-1+n)}^{h} = \Phi_{v,j-0.5,l-1}^{h-}, \qquad W_{2l+2n(j-1+n)}^{h} = \Phi_{v,j-0.5,l}^{h+},$$
(50)

such that matrices \mathbf{H}_h and \mathbf{D}_h have at least half of their non-vanishing elements concentrated close to the main diagonal; see schematic representation of these matrices in Fig. 6 for the case of n = 4. In the matrix \mathbf{H}_h , only the elements denoted by black or red stars are non-vanishing. In the easily invertible matrix \mathbf{D}_h , the elements denoted by black stars vanish as well, whereas at the positions of red stars stands 1. Once the algorithm is constructed correctly, calculating both matrix-vector products $\mathbf{H}_h V^h$ and $\mathbf{D}_h V^h$ requires $\sim 44n^2$ arithmetic operations; estimating $\mathbf{D}_h^{-1} V^h$ with arbitrary $4n^2$ dimensional vector V^h can be done with $\sim 4n^2$ operations. Construction of the whole matrix $\mathbf{D}_h^{-1} \mathbf{H}_h$ with $\sim 8n^3$ non-vanishing entries also requires $\sim 4n^2$ operations.

4.2 Example

For the construction and solution of the discrete spectral problem (45), we used Julia programming language (version 1.9) [3], all formulas and schemes presented above in this work, and the function "eigen()" available within the Julia's "LinearAlgebra" library. The example calculations presented in Fig. 7 were performed for the PCSEL device with $L = 300 \,\mu$ m (as considered in Ref. [6]), with the vertical structure and PC layer's configuration explored already when performing calculations for Figs. 2, 3, and 4. In this example, the modes (Λ_h, Φ^h) solve the discrete spectral problem (45) for several small-to-moderate discretization parameter n values.



Figure 7: Calculations of eigenvalues Λ_h solving Eq. (45). (a): All Λ_h for the cases n = 16 (magenta), 32 (red), and 48 (light blue). (b): same Λ_h close to the origin. (c) and (d): Convergence of the main (smallest threshold) and the second mode with growing n. Empty symbols (squares, circles, triangles, rhombs) in (b)-(d): five main modes for n = 48. Orange full squares in (a), (b): eigenvalues Λ_{1D} in the limit case of the original system (3) with decoupled Φ_u and Φ_v . Black triangle in (b): lowest-threshold eigenvalue of $i\mathbf{C}$. Bottom row diagrams: intensity distributions of five main identically scaled eigenfunctions, $|\Phi^h(x, y)|^2$, within $[0, L] \times [0, L]$.

The numerical scheme (45) has $4n^2$ (i.e., a finite number of) eigenvalues Λ_h and, thus, is not able to approximate all (an infinite number of) eigenvalues Λ of the original problem (3). Fig. 7(a) shows

how the spectra of (45) evolve with an increase of n. For each fixed n, most of the eigenvalues Λ_h belong to the prolongated clusters, all grouped along the circle whose radius is proportional to n (or 1/h, where h is a discrete mesh size in both spatial directions). The number of clusters and the number of modes within each cluster grows linearly with n. Eigenvalues Λ_h having large values of $-\Re\Lambda_h$ (at least 90% of the the upper part of "mode-circles") are far away from realistic Λ , which for an uncoupled Φ_u and Φ_v case are represented by densely to each other located orange squares in panel (a). On the other hand, eigenvalues Λ_h located on the lower part of the "mode circle" provide a much better resemblance of realistic Λ : see Fig. 7(b) where only Λ_h within a small window close to the origin are shown. We can see four clusters of (red and light blue) modes with an accumulation of Λ_h close to four orange boxes representing exact eigenvalues Λ_{1D} of Eq. (3) with the decoupled cross-propagating fields. Note also that whereas the tips of two lower clusters of magenta modes (calculated for a low n = 16) are still pretty well represented by Λ_{1D} , the remaining clusters are further apart, indicating an insufficient approximation of the corresponding modes at this low value of n.

Five main modes calculated with n = 48 are indicated by different empty black-framed symbols in the upper panels of Fig. 7. Their intensity distributions $|\Phi^h(x,y)|^2 = |\Phi_u^{h+}|^2 + |\Phi_u^{h-}|^2 + |\Phi_v^{h+}|^2 + |\Phi_v^{h+}|^2$ are presented in the bottom-row panels. While third-to-fifth low-threshold modes are close to the lowest Λ_{1D} in Fig. 7(b), two main modes belong to the mode group tending towards the filled black triangle, representing one of four eigenvalues $\Lambda_{i\mathbf{C}}$ of the matrix $i\mathbf{C}$ shown in Fig. 2(c). It is a significant coupling of the cross-propagating fields, which implies a significant separation of these two most important modes from Λ_{1D} . The suggested configuration of the PCSEL implies a wellpronounced mode threshold gap for these modes, and already small $n \sim 20$ can provide pretty good approximations for several critical eigenvalues Λ of the original spectral problem (3). The last statement is illustrated by Fig. 7(c) and (d), showing a convergence of Λ_h for two main modes with an increase of n (note the same scaling of both axes in these diagrams).

The sufficiency of low n would be a perfect message in practical computations since calculations of all Λ_h for n = 20 took about 2 minutes, while the same task using n = 40 was performed in more than 4 hours. Finally, we note that in the presented example we still used a moderate value of L suggested in Ref. [6]. However, our algorithms also work well for much larger structures with $L > 1000 \,\mu$ m, which will be considered when designing new PCSEL devices.

4.3 Higher order schemes

As it was mentioned earlier, the schemes above provide a second-order approximation w.r.t. the discretization step h. When dealing with larger PCSEL devices requiring finer discretizations and, thus, substantial memory resources and processing time, it could be helpful to explore higher-order schemes [1]. A reasonable fourth-order scheme can be realized by replacing pretty simple operators σ_k^h and $\sigma_k^{\dagger h}$ in Eq. (47) with more elaborated ones, acting differently for inner (1 < k < n) and boundary (k = 1, n) cells of the discretized domain:

$$\sigma_{k}^{h}V^{h} = \begin{cases} \frac{35V_{k-1}^{h} + 140V_{k}^{h} - 70V_{k+1}^{h} + 28V_{k+2}^{h} - 5V_{k+3}^{h}}{128} & \text{for } k = 1\\ \frac{9(V_{k}^{h} + V_{k-1}^{h}) - (V_{k+1}^{h} + V_{k-2}^{h})}{8} & \text{for } 1 < k < n \\ \frac{35V_{k}^{h} + 140V_{k-1}^{h} - 70V_{k-2}^{h} + 28V_{k-3}^{h} - 5V_{k-4}^{h}}{128} & \text{for } k = n \end{cases}$$

$$\sigma_{k}^{\dagger h}V^{h} = \begin{cases} \frac{-22V_{k-1}^{h} + 17V_{k}^{h} + 9V_{k+1}^{h} - 5V_{k+2}^{h} + V_{k+3}^{h}}{24h} & \text{for } k = 1\\ \frac{27(V_{k}^{h} - V_{k-1}^{h}) - (V_{k+1}^{h} - V_{k-2}^{h})}{24h} & \text{for } 1 < k < n \\ \frac{22V_{k}^{h} - 17V_{k-1}^{h} - 9V_{k-2}^{h} + 5V_{k-3}^{h} - V_{k-4}^{h}}{24h} & \text{for } k = n \end{cases}$$
(51)

These formulas are at least twice longer than those of (47), such that the corresponding matrices H_h and D_h in Eq. (49) have more non-vanishing elements now. Shorter expressions within the inner cells can be explained by the symmetry of the applied stencil w.r.t. the center of the cell where the approximation of the continuous functions and their derivatives is performed. In contrast, this symmetry is lost at the border cells, and the fourth-order approximations here use five mesh points. Loss of the symmetry also violates the conservation law (48). Similarly, one can also construct even higher 2s-order schemes (45), which are defined by further modifications of operators σ_k^h and $\sigma_k^{\dagger h}$ which exploit 2s + 1 values of the grid function at s - 1 outer cell layers, and 2s values of the same grid function within the remaining inner cells.



Figure 8: Comparison of schemes with different approximation orders used to calculate the five lowest threshold modes. Calculation time (a) and precision of calculated main (b) and the second (c) modes as functions of discretization parameter n. Dashed in (a): approximation of time by n^{ρ} .

The performance of different schemes is represented in Fig. 8. In contrast to our previous study shown in Fig. 2, where all eigenvalues Λ_h of the considered discrete problem (45) were calculated, now we calculated only five major modes but could exploit fine numerical meshes generated using $n \leq 512$ instead. Panel (a) of Fig. 8 shows the calculation time required to find these main modes using different approximations and discretization parameters n. In all cases, the simulation time grows with an increase of n as n^{ρ} , with ρ being between 2.3 and 2.9. We note a large gap between the times required by 2nd-order and 4th-order schemes compared to those of higher-order schemes. We attribute this difference to the trivial two-diagonal form of the matrix \mathbf{D}_h in the 2nd order scheme (red dots in Fig. 6), which is supplemented by additional diagonals and spoiled by the border-cell-induced asymmetries in the higher-order schemes.

Panels (b) and (c) of Fig. 8 show a convergence (i.e., decay of the absolute errors $|\Lambda_h - \Lambda|$) of two major eigenvalues with the up-sweep of n. "Exact" eigenvalues Λ in this study were calculated using n = 512 and the 8th-order scheme. The calculations due to 2nd and 4th-order schemes (magenta and green) show the expected convergence rate nicely. This rate for even higher order schemes is degraded once the error reaches $\sim 10^{-15}$, the level at which approximations of Λ_h in the iterative procedure used by the spectral solver could not be adequately distinguished anymore.

From a practical point of view, these diagrams clearly show the advantages of the higher-order schemes, even if for the same n, these schemes require up to 10 times longer calculation time. For example, the precision of 10^{-6} for the main mode, see panel (b), is achieved using $n \approx 100$ and 16 in the 2nd and 4th-order schemes, whereas the calculation time for these cases, see panel (a), is about 1 and 0.03 seconds, respectively. Since the higher-order precision schemes do not demand very fine meshes, one can use them for reliable estimation of the main modes in large-area PCSELs with L in the mm-cm range.

5 Conclusion

In this work, we addressed the practical problems arising during the construction of the mathematical model for novel PCSEL devices, which, up to our knowledge, were not discussed yet in the (mainly engineering) papers on PCSELs. Namely, we gave a detailed description of the algorithms to construct the field cross-coupling matrices C, indicated possible numerical problems related to the limitations of computer arithmetics when dealing with the huge and tiny values of the exponential functions, and presented methods for avoiding these limitations. Our algorithms for constructing C rely on analytic formulas. They are precise and much more efficient than fully numerical approaches and allow us to account for a much larger number of submatrices $\mathbf{C}_{2D}^{(r,s)}$ in the infinite series used for the definition of C_{2D} and C. Next, we constructed the 2nd-order finite difference scheme for the spectral problem. After deriving a discrete analog of the integral conservation law, we demonstrated the performance of this scheme in solving the spectral problem for a selected PCSEL device. We have shown that even the schemes with relatively coarse numerical meshes can provide decent approximations of several main eigenvalues of the original problem. Finally, we have also constructed the higher order schemes, which can be preferable if a better precision of calculated spectra is required, many similar spectral calculations should be performed in a limited time, or spectral calculations of PCSELs with a huge emission area (large L) are needed.

References

- [1] N.S. Bakhvalov, G.M. Kobel'kov and N.P. Zhidkov. *Chislennye metody*. Fizmatlit, Moscow, 2000. in Russian
- [2] M.J. Bergmann and H.C. Casey. Optical-field calculations for lossy multiple-layer $Al_xGa_{1-x}N/In_xGa_{1-x}N$ laser diodes. *J. of Appl. Phys.*, **84**(3):1196–1203, 1998.
- [3] J. Bezanson, A. Edelman, S. Karpinski and V.B. Shah. Julia: A fresh approach to numerical computing. *SIAM review*, **59**(1):65–98, 2017. doi: 10.1137/141000671.
- [4] J. Chilwell and I. Hodgkinson. Thin-films field-transfer matrix theory of planar multilayer waveguides and reflection from prism-loaded waveguides. J. Opt. Soc. Am. A, 1(7):742–753, 1984. doi: 10.1364/JOSAA.1.000742.
- [5] M. Imada, S. Noda, A. Chutinan, T. Tokuda, M. Murata and G. Sasaki. Coherent two-dimensional lasing action in surface-emitting laser with triangular-lattice photonic crystal structure. *Appl. Phys. Lett.*, **75**:316–318, 1999. doi: 10.1063/1.124361.
- [6] T. Inoue, R. Morita, M. Yoshida, M. De Zoysa, Y. Tanaka and S. Noda. Comprehensive analysis of photonic-crystal surface-emitting lasers via time-dependent three-dimensional coupled-wave theory. *Physical Review B*, **99**:035308, 2019. doi: 10.1103/PhysRevB.99.035308.
- [7] Y. Liang, C. Peng, K. Sakai, S. Iwahashi and S. Noda. Three-dimensional coupled-wave analysis for square-lattice photonic crystal surface emitting lasers with transverse-electric polarization: finite-size effects. *Optics Express*, **20**(14):15945–15961, 2012. doi: 10.1364/OE.20.015945.
- [8] C. Peng, Y. Liang, K. Sakai, S. Iwahashi and S. Noda. Coupled-wave analysis for photonic-crystal surface-emitting lasers on air holes with arbitrary sidewalls. *Opt. Express*, **19**(24):24672–24686, 2011. doi: 10.1364/OE.19.024672.

- [9] J. Piprek(Ed.). *Optoelectronic Devices Advanced Simulation and Analysis*, chapter Multisection Lasers: Longitudinal Modes and their Dynamics, pp. 121–150. Springer, New York, 2005.
- [10] M. Radziunas and R. Čiegis. Effective numerical algorithm for simulations of beam stabilization in broad area semiconductor lasers and amplifiers. *Math. Model. Anal.*, **19**(5):627–646, 2014. doi: 10.3846/13926292.2014.979453.
- [11] M. Yoshida, S. Katsuno, T. Inoue, J. Gelleta, K. Izumi, M. De Zoysa, K. Ishizaki and S. Noda. Highbrightness scalable continuous-wave single-mode photonic-crystal laser. *Nature*, **618**:727–732, 2023. doi: 10.1038/s41586-023-06059-8.
- [12] A. Zeghuzi, M. Radziunas, H.-J. Wünsche J.-P. Koester, H. Wenzel, U. Bandelow and A. Knigge. Traveling wave analysis of non-thermal far-field blooming in high-power broad-area lasers. *IEEE J. of Quantum Electronics*, 55(2):2000207, 2019. doi: 10.1109/JQE.2019.2893352.
- [13] A. Zeghuzi, H.-J. Wünsche, H. Wenzel, M. Radziunas, J. Fuhrmann, A. Klehr, U. Bandelow and A. Knigge. Time-dependent simulation of thermal lensing in high-power broad-area semiconductor lasers. *IEEE J. of Selected Topics in Quantum Electronics*, 25(6):1502310, 2019. doi: 10.1109/JSTQE.2019.2925926.