A Bloch mode expansion approach for analyzing quasi-normal modes in open nanophotonic structures

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Abstract

We present a new method for determining quasi-normal modes in open nanophotonic structures using a modal expansion technique. The outgoing wave boundary condition of the quasi-normal modes is satisfied automatically without absorbing boundaries, representing a significant advantage compared to conventional techniques. The quasi-normal modes are determined by constructing a cavity roundtrip matrix and iterating the complex mode wavelength towards a unity eigenvalue. We demonstrate the method by determining quasi-normal modes of cavities in two-dimensional photonic crystals side-coupled to W1 waveguides.

1. Introduction

In micro- and nanostructured media, such as micropillars and photonic crystals (PhCs), characteristic feature sizes are on the order of the wavelength of light which makes analysis of light propagation in these systems intricate. Design of such structures therefore relies on an interplay between theory, computations and fabrication, and to avoid analysis and design based on trial-and-error transparent and efficient numerical methods are indispensable. In open structures, the natural modes are so-called quasi-normal modes which are solutions to the frequency domain wave equation satisfying an outgoing wave boundary condition (BC) [1]. Numerical modeling often includes artificial BCs to ensure finite-sized computation domains, needed to handle the computations in computers. Simple choices include Dirichlet and periodic BCs that give rise to normal modes which, however, suffer from parasitic reflections at the artificial boundaries. These unwanted effects can to some extent be suppressed by means of absorbing boundaries like perfectly matched layers (PMLs) [2], but their implementation remains problematic, in particular in geometries featuring infinite periodic structuring like PhCs. The outgoing wave BC is thus difficult to satisfy with conventional spatial discretization techniques like the finite-difference time-domain (FDTD) method and the finite element method (FEM) due to their need for absorbing BCs.

In this work, we present a new method for determining quasi-normal modes using a modal expansion method [3, Chap. 6], a scattering matrix approach [4] and Bloch modes of periodic structures [5, Chap. 3]. In Fig. 1, two quasi-normal modes in two-dimensional PhC cavities are displayed. Light propagates in the z-direction, and as detailed in the following sections the outgoing wave BC in this direction is satisfied automatically; this represents a significant advantage of the new method.

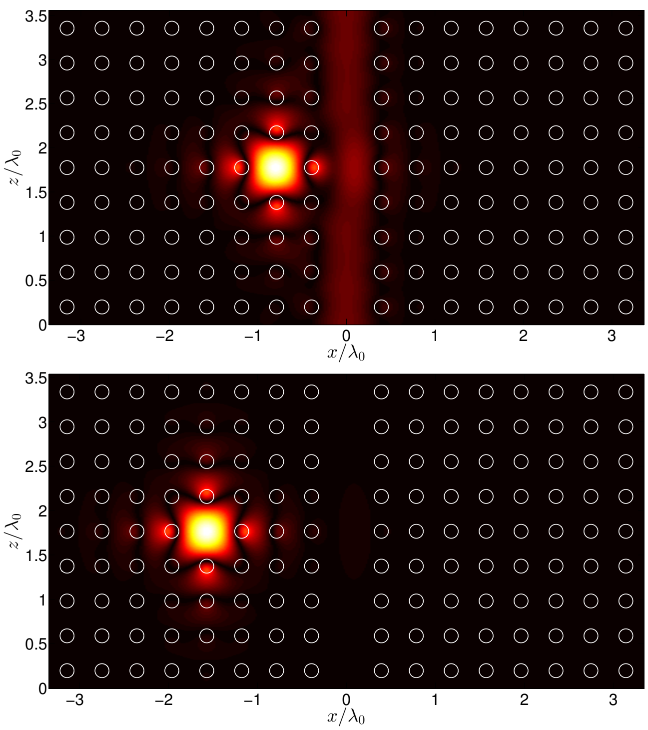

Figure 1: Quasi-normal mode field distribution ($|E_y|$ [a.u.]) in cavity side-coupled to W1 waveguide in two-dimensional rectangular lattice PhC. The complex mode wavelengths are $\lambda_0/a = 2.53 + 0.0087\mathrm{i}$ (top panel) and $\lambda_0/a = 2.55 + 0.000064\mathrm{i}$ (bottom panel), with $a = 0.4\,\mu\mathrm{m}$ being the PhC lattice constant and $\epsilon_{\mathrm{Rods}} = 8.9$ and $\epsilon_{\mathrm{Back}} = 1$.

2. Bloch mode expansions and quasi-normal modes

2.1. Bloch modes and scattering matrices

In the modal expansion technique used here [3, Chap. 6], the structure to be analyzed is sliced into periodic sections along a chosen propagation direction, taken here as the z-direction. The periodicity along z, with period a, implies that the electromagnetic fields in each section w can be expanded on Bloch modes $\mathbf{e}_j^w(\mathbf{r}_\perp, z)$,

$$\mathbf{E}^w(\mathbf{r}) = \sum_j c_j^w \mathbf{e}_j^w(\mathbf{r}_\perp, z), \quad (1)$$

that are quasi-periodic functions of the z-coordinate [5, Chap. 3]

$$\mathbf{e}_j^w(\mathbf{r}_\perp, z + a^w) = \exp(\mathrm{i}k_j^w a^w)\mathbf{e}_j^w(\mathbf{r}_\perp, z), \quad (2)$$

where k_j^w is the wavenumber of the jth Bloch mode. This wavenumber is purely real for a propagating Bloch mode while inside a bandgap it has a finite imaginary part giving rise to exponentially decaying waves. For uniform sections, like translation invariant ridge waveguides, the Bloch modes become the well-known waveguide modes, but the description using the more general Bloch modes provides a powerful framework for analyzing, for example, PhCs. The Bloch mode form in Eq. (2) holds the analytic z-dependence of the electromagnetic fields, and this is what allows to satisfy the outgoing wave BC of the quasi-normal modes in the z-direction without using artificial BCs. In Eq. (1), c_j^w are expansion coefficients determined to satisfy the electromagnetic BCs across section interfaces. This is handled using a scattering matrix formalism [4], which in particular relates the incoming and outgoing Bloch mode amplitudes via the total scattering matrix $\mathbf{S}$

$$\mathbf{c}_{\mathrm{out}} = \mathbf{S}\mathbf{c}_{\mathrm{in}}. \quad (3)$$

2.2. Quasi-normal modes

It has been suggested that quasi-normal modes in nanophotonic structures can be calculated as non-zero solutions $\mathbf{c}_{\mathrm{out}}$ of Eq. (3) for a vanishing input $\mathbf{c}_{\mathrm{in}} = \mathbf{0}$ [6, 7]. This yields the following equation

$$\mathbf{S}^{-1}(\lambda_0)\mathbf{c}_{\mathrm{out}} = \mathbf{0}, \quad (4)$$

where we have written the wavelength dependence of the inverse scattering matrix explicitly. This equation, in general, only has non-trivial solutions at complex values of λ_0, the quasi-normal mode complex wavelength. The search for these complex wavelengths is in principle straightforward, but for advanced structures that require the inclusion of a large number of modes the associated scattering matrix is comparatively large, and the construction of the inverse scattering matrix in Eq. (4) may be complicated and unstable.

In this context, we suggest a new and simpler formulation for determining the quasi-normal modes. For a given structure, the relevant cavity section w_{c} is identified, and the cavity roundtrip matrix [8] $\mathbf{M}^{w_{\mathrm{c}}}$ is constructed

$$\mathbf{M}^{w_{\mathrm{c}}}(\lambda_0) \equiv \mathbf{R}^{\mathrm{bot}}\mathbf{P}_-^{w_{\mathrm{c}}}\mathbf{R}^{\mathrm{top}}\mathbf{P}_+^{w_{\mathrm{c}}}, \quad (5)$$

where $\mathbf{R}^{\mathrm{bot}}$ ($\mathbf{R}^{\mathrm{top}}$) is the scattering reflection matrix between the cavity section and the bottommost (topmost) section. $\mathbf{P}_+^{w_{\mathrm{c}}}$ and $\mathbf{P}_-^{w_{\mathrm{c}}}$ are diagonal matrices accounting for the propagation of the Bloch modes through the cavity section.

At real wavelengths, the eigenvalues of $\mathbf{M}^{w_{\mathrm{c}}}$ have absolute values below unity since the reflectivities of the mirrors surrounding the cavity section are smaller than unity; in every roundtrip, a fraction of the light leaks out of the cavity and into the mirrors. However, by analytically continuing the definition of $\mathbf{M}^{w_{\mathrm{c}}}$ into the complex wavelength plane it is possible to compensate the mirror losses by making the elements in the propagation matrices $\mathbf{P}_+^{w_{\mathrm{c}}}$ and $\mathbf{P}_-^{w_{\mathrm{c}}}$ larger than unity. We therefore iterate the complex wavelength λ_0 to find an eigenvalue of $\mathbf{M}^{w_{\mathrm{c}}}$ equal to unity; the associated eigenvector gives the quasi-normal mode distribution in the cavity section

$$\mathbf{M}^{w_{\mathrm{c}}}(\lambda_0)\mathbf{c}^{w_{\mathrm{c}}} = \mathbf{c}^{w_{\mathrm{c}}}. \quad (6)$$

The finite imaginary part of the quasi-normal mode wavelength gives rise to a finite Q-factor of the mode [9, Chap. 11]

$$Q = \frac{\mathrm{Re}(\lambda_0)}{2\mathrm{Im}(\lambda_0)}, \quad (7)$$

and also means that the quasi-normal modes diverge when propagating outwards; this renders the associated mode volume non-trivial to calculate [10, 11].

3. Example: W1 waveguide and side-coupled cavity in rectangular lattice photonic crystal

We consider two-dimensional structures that are uniform and infinitely extended in the y-direction. In this case, Maxwell's equations decouple into TE- and TM-polarizations in which the fields may be described completely by the scalars E_y and H_y, respectively. We focus on two-dimensional rectangular lattice PhCs with dielectric rods ($\epsilon_{\mathrm{Rods}} = 8.9$) suspended in free-space ($\epsilon_{\mathrm{Back}} = 1$). This structure is known to possess a TE-bandgap [5, Chap. 5], with the electric field having only its y-component E_y non-zero. By removing one row of holes a W1 waveguide is created, and for wavelengths inside the bandgap light may be guided through this waveguide. By furthermore removing one rod in the bulk of the PhC lattice and in the vicinity of the waveguide a cavity is formed, see Fig. 1; we here focus on determining the quasi-normal modes of this structure.

We first crudely locate the quasi-normal mode spectrally by calculating the transmission of the guided Bloch mode through the structure; a dip in the transmission spectrum indicates the excitation of the cavity mode. Subsequently, we use the spectral position of the transmission minimum as a starting point for the iteration using a Newton-Raphson algorithm towards a complex wavelength that gives an eigenvalue of unity for $\mathbf{M}^{w_{\mathrm{c}}}(\lambda_0)$. We do the above for two positions of the cavity; separated by one rod and by three rods from the waveguide. The quasi-normal mode distributions ($|E_y|$) are shown in the top and bottom panels of Fig. 1, respectively, and the associated quasi-normal mode wavelengths are $\lambda_0/a = 2.53 + 0.0087\mathrm{i}$ and $\lambda_0/a = 2.55 + 0.000064\mathrm{i}$, respectively, with $a = 0.4\,\mu\mathrm{m}$ being the PhC lattice constant. We note that both modes have roughly the same real part of the mode wavelength, while the imaginary part decreases as the cavity is moved further away from the waveguide. Using Eq. (7), the Q-factors are found to be $Q = 145$ (top panel) and $Q = 19820$ (bottom panel), and for this structure we gain approximately an order of magnitude in Q when the cavity is moved a lattice constant away from the waveguide.

We have tested the method with other structures that exhibit lower Q-factors, and this in general challenges the numerical stability of the formalism since it corresponds to wavelengths with comparatively large imaginary parts. We have, however, been able to determine modes with Q as low as 25, and this demonstrates that the method can be useful for plasmonic structures, that usually feature low-Q modes, as well.

4. Conclusion

We have proposed a new method for determining quasi-normal modes in open nanophotonic structures using a Bloch mode expansion approach. The scheme relies on an iteration of the complex quasi-normal mode wavelength to determine a unity eigenvalue of the cavity section roundtrip matrix. The unity eigenvalue approach is analogous to the lasing condition in laser cavities and is thus more intuitive, more efficient and simpler than other methods that rely on inversion of the total scattering matrix. The use of modal expansion techniques to determine quasi-normal modes as compared to conventional techniques like FDTD and the FEM is advantageous since the outgoing wave BC of the quasi-normal modes can be satisfied automatically and without artificial absorbing boundaries. We have demonstrated the use of our method by determining quasi-normal modes in side-coupled cavities in two-dimensional rectangular lattice PhCs, and we have discussed the effect of the cavity position with respect to a nearby W1 waveguide on the quasi-normal mode Q-factor.

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References

[1] P. T. Kristensen and S. Hughes, "Modes and mode volumes of leaky optical cavities and plasmonic nanoresonators," *ACS Photonics*, vol. 1, no. 1, pp. 2–10, 2014.

[2] J.-P. Berenger, "A perfectly matched layer for the absorption of electromagnetic waves," *J. Comput. Phys.*, vol. 114, no. 2, pp. 185–200, Oct 1994.

[3] A. V. Lavrinenko, J. Lægsgaard, N. Gregersen, F. Schmidt, and T. Søndergaard, *Numerical Methods in Photonics*. CRC Press, 2014.

[4] L. Li, "Formulation and comparison of two recursive matrix algorithms for modeling layered diffraction gratings," *J. Opt. Soc. Am. A*, vol. 13, no. 5, pp. 1024–1035, May 1996.

[5] J. Joannopoulos, S. Johnson, J. Winn, and R. Meade, *Photonic Crystals: Molding the Flow of Light*, 2nd ed. Princeton University Press, 2011.

[6] T. Weiss, N. A. Gippius, S. G. Tikhodeev, G. Granet, and H. Giessen, "Derivation of plasmonic resonances in the Fourier modal method with adaptive spatial resolution and matched coordinates," *J. Opt. Soc. Am. A*, vol. 28, no. 2, pp. 238–244, Feb 2011.

[7] D. A. Bykov and L. L. Doskolovich, "Numerical methods for calculating poles of the scattering matrix with applications in grating theory," *J. Lightwave Technol.*, vol. 31, no. 5, pp. 793–801, Mar 2013.

[8] N. Gregersen, S. Reitzenstein, C. Kistner, M. Strauss, C. Schneider, S. Höfling, L. Worschech, A. Forchel, T. Nielsen, J. Mørk, and J.-M. Gérard, "Numerical and experimental study of the Q factor of high-Q micropillar cavities," *IEEE J. Quant. Electron.*, vol. 46, no. 10, pp. 1470–1483, Oct 2010.

[9] L. Novotny and B. Hecht, *Principles of Nano-Optics*, 2nd ed. Cambridge University Press, 2012.

[10] P. T. Kristensen, C. V. Vlack, and S. Hughes, "Generalized effective mode volume for leaky optical cavities," *Opt. Lett.*, vol. 37, no. 10, pp. 1649–1651, May 2012.

[11] C. Sauvan, J. P. Hugonin, I. S. Maksymov, and P. Lalanne, "Theory of the spontaneous optical emission of nanosize photonic and plasmon resonators," *Phys. Rev. Lett.*, vol. 110, p. 237401, Jun 2013.