A Bloch modal approach for engineering waveguide and cavity modes in two-dimensional photonic crystals

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ABSTRACT

In open nanophotonic structures, the natural modes are so-called quasi-normal modes satisfying an outgoing wave boundary condition. We present a new scheme based on a modal expansion technique, a scattering matrix approach and Bloch modes of periodic structures for determining these quasi-normal modes. As opposed to spatial discretization methods like the finite-difference time-domain method and the finite element method, the present approach satisfies automatically the outgoing wave boundary condition in the propagation direction which represents a significant advantage of our new method. The scheme uses no external excitation and determines the quasi-normal modes as unity eigenvalues of the cavity roundtrip matrix. We demonstrate the method and the quasi-normal modes for two types of two-dimensional photonic crystal structures, and discuss the quasi-normal mode field distributions and Q-factors in relation to the transmission spectra of these structures.

Keywords: Bloch modes, quasi-normal modes, photonic crystals, waveguides, cavities, modal expansion techniques.

1. INTRODUCTION

In open nanophotonic structures, the natural modes are so-called quasi-normal modes that are solutions to the frequency domain wave equation with an outgoing wave boundary condition (BC).[1] Numerical modeling of such structures 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 photonic crystals (PhCs). The outgoing wave BC is thus difficult to satisfy with conventional spatial discretization techniques like the finite-difference time-domain (FDTD)[3] method and the finite element method (FEM)[4] due to their need for absorbing BCs.

In this work, we present a new method for determining quasi-normal modes using a modal expansion technique,[5] a scattering matrix approach[6] and Bloch modes of periodic structures.[7] The paper is organized as follows: Section 2 outlines the procedure for determining the quasi-normal modes, Section 3 provides numerical examples of quasi-normal modes in two different PhC structures, and Section 4 concludes the work and provides an outlook for future work.

In Fig. 1, four quasi-normal modes in two-dimensional PhC cavities are displayed (more details in Section 3). Light propagates in the z-direction, and as detailed in the following section the outgoing wave BC in this direction is satisfied automatically; this represents a significant advantage of the new method.

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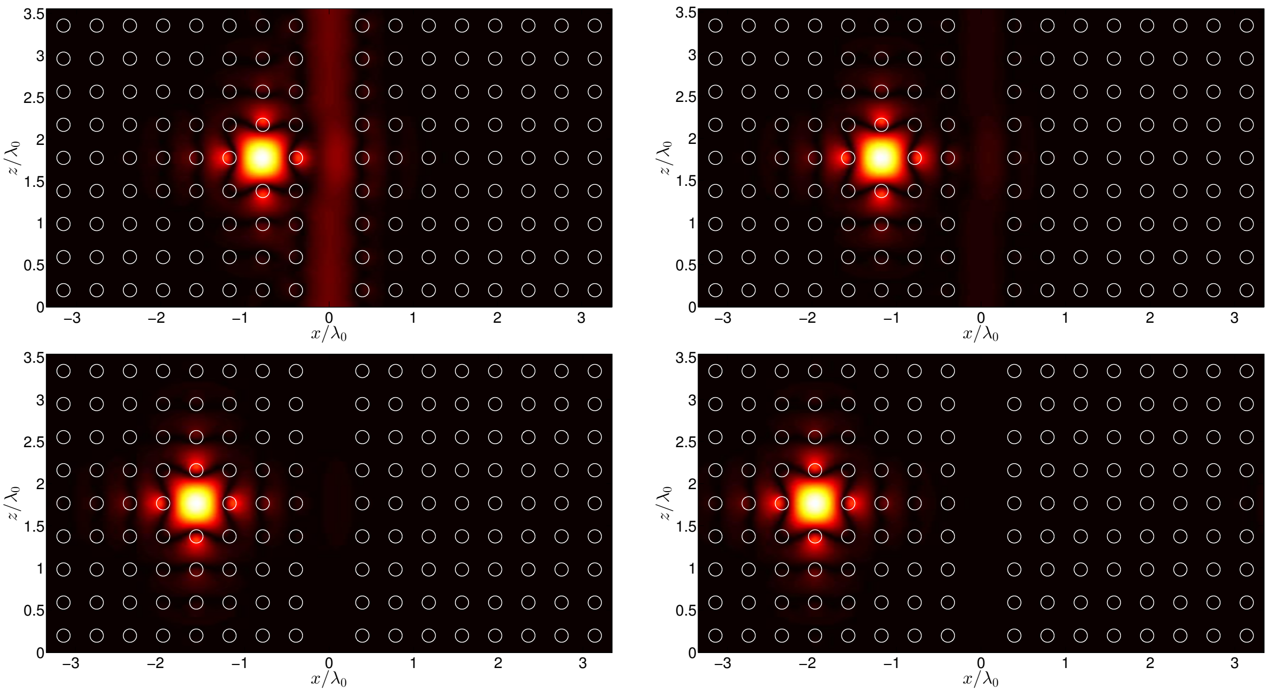

Figure 1. Quasi-normal mode field distribution ($|E_y|$ [a.u.]) in cavity side-coupled to W1 waveguide in two-dimensional rectangular lattice PhC. The associated quasi-normal mode wavelengths and Q-factors are given in Table 1.

2. BLOCH MODE EXPANSIONS AND QUASI-NORMAL MODES

2.1 Bloch modes and scattering matrices

In the modal expansion technique used here,[5] 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 $\mathbf{e}_j^w(\mathbf{r}_\perp, z)$,

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

that are quasi-periodic functions of the z-coordinate[7]

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

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,[6] which in particular relates the incoming and outgoing Bloch mode amplitudes via the total scattering matrix $\mathbf{S}$

$$\mathbf{c}_{\text{out}} = \mathbf{S}\mathbf{c}_{\text{in}}. \tag{3}$$

2.2 Quasi-normal modes

It has been suggested that quasi-normal modes in nanophotonic structures can be calculated as non-zero solutions $\mathbf{c}_{\text{out}}$ of Eq. (3) for a vanishing input $\mathbf{c}_{\text{in}} = \mathbf{0}$.[8,9] This yields the following equation

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

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[10] $\mathbf{M}^{w_c}$ is constructed

$$\mathbf{M}^{w_c}(\lambda_0) \equiv \mathbf{R}^{\text{bot}}\mathbf{P}_-^{w_c}\mathbf{R}^{\text{top}}\mathbf{P}_+^{w_c}, \tag{5}$$

where $\mathbf{R}^{\text{bot}}$ ($\mathbf{R}^{\text{top}}$) is the scattering reflection matrix between the cavity section and the bottommost (topmost) section. $\mathbf{P}_+^{w_c}$ and $\mathbf{P}_-^{w_c}$ are diagonal matrices accounting for the propagation of the Bloch modes through the cavity section. At real wavelengths, the eigenvalues of $\mathbf{M}^{w_c}$ 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 $\mathbf{M}^{w_c}$ into the complex wavelength plane it is possible to compensate the mirror losses by making the elements in the propagation matrices $\mathbf{P}_+^{w_c}$ and $\mathbf{P}_-^{w_c}$ larger than unity. We therefore iterate the complex wavelength λ_0 to find an eigenvalue of $\mathbf{M}^{w_c}$ equal to unity; the associated eigenvector gives the quasi-normal mode field distribution in the cavity section

$$\mathbf{M}^{w_c}(\lambda_0)\mathbf{c}^{w_c} = \mathbf{c}^{w_c}. \tag{6}$$

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

$$Q = \frac{\text{Re}(\lambda_0)}{2\text{Im}(\lambda_0)}, \tag{7}$$

and also means that the quasi-normal modes diverge when propagating outwards; this renders the associated mode volume non-trivial to calculate.[12,13]

3. QUASI-NORMAL MODES IN PHOTONIC CRYSTALS

In the following sections, we calculate and discuss quasi-normal modes in two types of photonic crystal structures. While the formalism for determining quasi-normal modes applies in any dimension, we consider two-dimensional (2D) structures that are assumed uniform and infinitely extended in the y-direction; in this case, Maxwell's equations decouple into TE- and TM-modes where the fields may be described fully by the scalars H_y and E_y, respectively. We focus on a rectangular lattice PhC, with high-index rods ($\epsilon_{\text{Rods}} = 8.9$) suspended in free-space ($\epsilon_{\text{Back}} = 1$). This structure is known to possess a TM-bandgap,[14] and by removing a row of rods we form a W1 waveguide in which light may be guided for wavelengths inside the bandgap of the bulk PhC. On top of the W1 waveguide, we add a side-coupled cavity in Section 3.1 (structure illustrated in Fig. 1) and in Section 3.2 additionally a blocking element in the waveguide (structure illustrated in inset in Fig. 2).

3.1 W1 waveguide and side-coupled cavity in rectangular lattice photonic crystal

In this section, we remove one rod in the bulk of the rectangular lattice PhC and thus form a cavity in the vicinity of the W1 waveguide. Computing the transmission of the guided Bloch mode through the waveguide and past the cavity as a function of wavelength, we observe a sharp dip around a central wavelength (full curve in Fig. 2). At this central wavelength, the cavity works as a highly reflecting mirror, and we associate the transmission dip with the excitation of a quasi-normal mode. For four different distances between the (center of the) W1 waveguide and the (center of the) cavity, we determine these quasi-normal modes; their field distributions ($|E_y|$) are shown in Fig. 1, with increasing cavity-waveguide distance from left to right and from top to bottom. The quasi-normal mode complex wavelengths and Q-factors are given in Table 1.

Considering first the real parts of the quasi-normal mode wavelengths $\text{Re}\,(\lambda_0)$, these essentially remain constant as the cavity is moved further into the bulk of the PhC. In contrast, the imaginary part $\text{Im}\,(\lambda_0)$ decreases by more than an order of magnitude when the cavity-W1 distance is increased by a lattice constant, and via Eq. (7) this

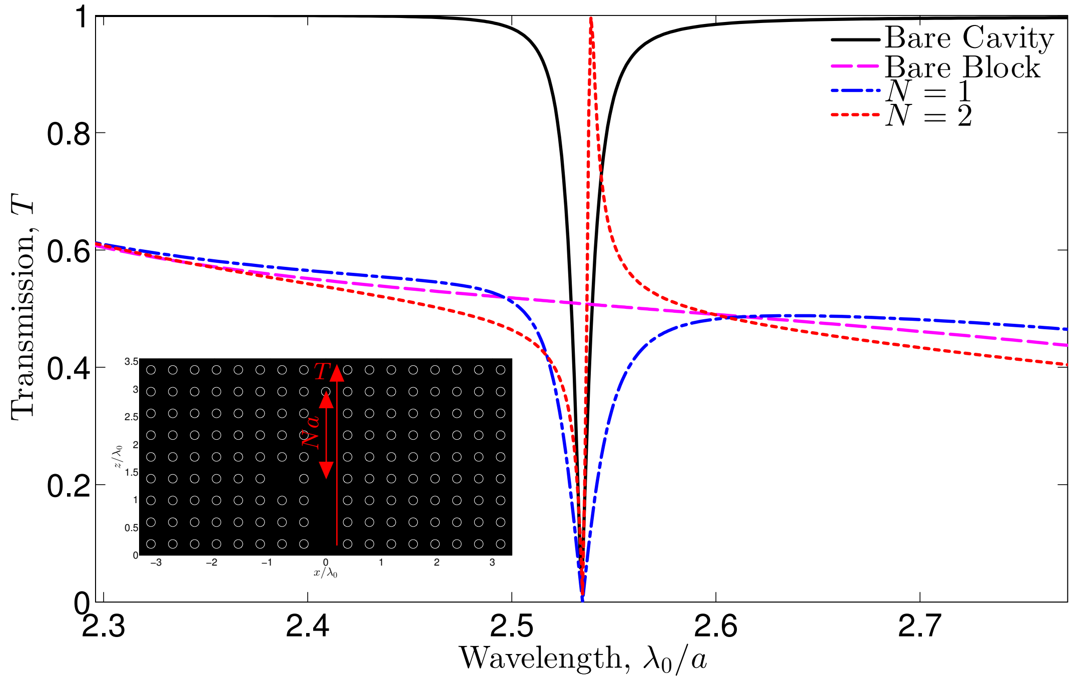

Figure 2. Transmission of guided Bloch mode as function of wavelength through PhC structure consisting of a W1 waveguide, a side-coupled cavity and a blocking rod in the middle of the waveguide. As shown in the inset, the distance between the cavity and the blocking element Na is a parameter. Spectra for the bare cavity (full), bare block (dashed), $N = 1$ (dotted-dashed) and $N = 2$ (dotted) are shown.

Fig. 1	Cavity-W1 distance $[a]$	$\mathrm{Re}(\lambda_0)$ $[a]$	$\mathrm{Im}(\lambda_0)$ $[a]$	Q
Top left	2	2.53	0.0087	$1.5 \cdot 10^2$
Top right	3	2.55	0.00078	$1.6 \cdot 10^3$
Bottom left	4	2.55	0.000064	$2.0 \cdot 10^4$
Bottom right	5	2.55	0.0000052	$2.4 \cdot 10^5$

Table 1. Quasi-normal mode wavelengths and Q-factors for cavity side-coupled to W1 waveguide structure; the associated quasi-normal mode field distributions are shown in Fig. 1.

produces quasi-normal mode Q-factors that increase by more than an order of magnitude when the distance is increased by a lattice constant. As compared to three-dimensional (3D) PhCs, these Q-factors do not include the out-of-plane contribution, but extending the mode expansion formalism to 3D structures[15] quasi-normal modes and their associated Q-factors can be determined to account for this as well.

Q-factors are typically obtained by resolving, for example, transmission spectra finely around a minimum or maximum to estimate the width of the Lorentzian shaped spectra. This requires calculations at many frequencies which is computationally demanding in advanced structures like PhCs. In turn, the quasi-normal mode determination only requires a few iterations of their complex mode wavelength to satisfy Eq. (6), yielding the Q-factors with much less effort.

3.2 Rectangular lattice Fano resonance photonic crystal

In the previous section, we observed the quasi-normal modes associated with the side-coupled cavity in the vicinity of a W1 waveguide in the rectangular lattice PhC. In this section, we fix the cavity-W1 distance to $2a$ and add a rod at a distance Na from the cavity in the middle of the W1 waveguide; see the inset in Fig. 2. This blocking element is partially reflecting, with a transmission of approximately 50-60% over the entire bandgap of the bulk

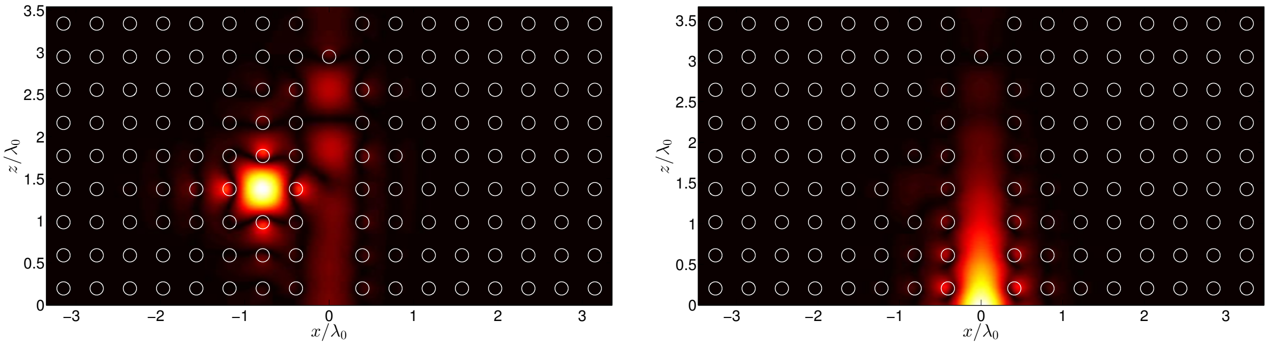

Figure 3. Quasi-normal mode field distributions ($|E_y|$ [a.u.]) in cavity side-coupled to W1 waveguide with a blocking element in a two-dimensional rectangular lattice PhC. The associated quasi-normal mode wavelengths and Q-factors are given in Table 2.

Fig. 3	$\mathrm{Re}(\lambda_0)$ $[a]$	$\mathrm{Im}(\lambda_0)$ $[a]$	Q
Left	2.54	0.0060	212
Right	2.46	0.23	5.4

Table 2. Quasi-normal mode wavelengths and Q-factors for cavity side-coupled to W1 waveguide with a blocking element structure; the associated quasi-normal mode field distributions are shown in Fig. 3.

PhC (dashed curve in Fig. 2). This type of structure has been proposed for optical switching since it may give rise to Fano shaped spectra and thus sharp spectral transitions between no transmission and full transmission.[16]

At $N = 1$ the transmission spectrum (dotted-dashed curve in Fig. 2) looks essentially like the product of the bare cavity and bare block spectra. In turn, at $N = 2$ the spectrum (dotted curve in Fig. 2) exhibits a Fano line shape, with a sharp shift from no transmission to full transmission around the bare cavity quasi-normal mode wavelength (compare this position of λ_0/a to the values of $\mathrm{Re}(\lambda_0)/a$ in Table 1). The Fano line shape occurs due to the interplay between a spectrally narrow and a spectrally broad mode, and the exact shape of the resulting spectrum depends sensitively on the relative phase between these two modes.[17]

With $N = 4$, these two quasi-normal modes look as shown in Fig. 3; the left panel shows the high-Q ($Q = 212$) cavity mode, while the right panel shows the low-Q ($Q = 5.4$) waveguide mode. In the left panel, a standing wave pattern is observed between the cavity and the blocking element, and in the right panel the quick divergence of the quasi-normal mode is apparent, stemming from the high value of $\mathrm{Im}(\lambda_0)$ of this mode. The determination of a low-Q quasi-normal mode as in the right panel of Fig. 3 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. Likewise, we have determined quasi-normal modes in two-dimensional rectangular lattice PhCs exhibiting Fano line shaped transmission spectra, and we have discussed the quasi-normal modes in the context of these transmission spectra. As an outlook, quasi-normal modes may constitute a rigorous basis for modeling light propagation in complex nanophotonic structures, and they have already been used to predict the dynamics in PhC structures.[18]

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