Multimodal Semi-analytical Model for Bound States in the Continuum and Unidirectional Guided Resonances in a Photonic Crystal

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Abstract. Recent attention has been directed towards optical bound states in the continuum (BICs) within photonic crystal slabs. Unidirectional guided resonances (UGRs) have also garnered interest, an associated phenomenon that involves intentionally broken symmetry and resulting in directional leakage. This study introduces a microscopic semi-analytical model to better understand these resonances. Building on a multimodal interference method used for BIC exploration, our approach extends to investigating UGRs, providing valuable insights into their distinct properties. Using this model, we aim to contribute to the design and comprehension of BICs and UGRs in photonic crystal slabs.

Keywords: BIC · photonic crystal · symmetry breaking

1 Introduction

In the last decade, the investigation of bound states in the continuum (BICs) has garnered significant attention because of their distinctive characteristics. Unlike typical confined modes, BICs exist alongside the radiation continuum, decoupling from it, and showcasing potential applications in areas such as spintronics, nanocavities, low-threshold lasing, sensing, and communication [1]. A closely related resonance, termed unidirectional guided resonance (UGR) [2], has recently been investigated. UGRs manifest in similar structures as BICs but exhibit broken symmetry, allowing radiation to leak exclusively in only one direction.

Various mechanisms explain the emergence of BICs, with the multimodal interference model being one such approach [3]. This model entails the interference of multiple fundamental modes, leading to destructive interference outside the structure and the creation of a BIC under specific conditions. This study demonstrates the applicability of the multimodal interference model to UGRs, offering a semi-analytical description of these

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resonances. This adaptability enables efficient exploration and interpretation of diverse geometries, providing valuable insights into UGR behavior and potential applications in photonic devices.

2 Method and Structure

The method employs multiple steps. First, we divide the crystal unit cell (Fig. 1a) into two halves, a top and bottom half (Fig. 1b), and create an infinite waveguide with the same dimension as the cell where it was cut (Fig. 1c). Subsequently, we calculate the dispersion of the infinite waveguide, providing insight into the coexisting modes in the vertical direction of the structure (Fig. 1d). Using a boundary mode analysis within the COMSOL simulation software, these modes are introduced into the two halves of the structure. This process enables the computation of two half-trip matrices, namely S_u for the upper part and S_d for the lower part, illustrating how the modes are reflected and mixed by the interfaces of the structure.

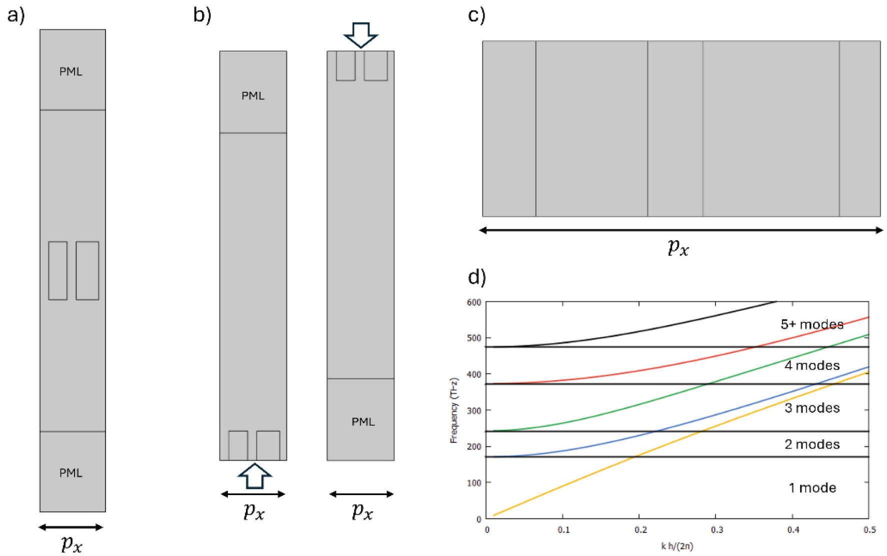

Fig. 1. a) The full unit cell of a photonic crystal, with period p_x along the horizontal direction (x). b) The two halves of the cell used to compute the half-trip matrices. c) A section of the waveguide that is infinite along the vertical direction (y). $p_x = 408$ nm, the width of the largest particle is 140 nm. The width of the smallest particle is varied to possibly break the symmetry between the two particles. The height is the same for the two particles and can be varied analytically via the propagation matrices (in this figure $L = 360$ nm). d) The TE (transverse electric) dispersion for the structure of c). Depending on the frequency, a different number of guided modes are available.

By combining the two half-trip matrices, we construct the round-trip matrix $S_d \times S_u$ which we then analyze by computing its eigenvalues and eigenvectors, similar as in Ref. [4]. For a system with 3 modes, one thus obtains:

$$S_d \times S_u \begin{bmatrix} C1 \\ C2 \\ C3 \end{bmatrix} = \lambda \begin{bmatrix} C1 \\ C2 \\ C3 \end{bmatrix}$$

This gives valuable information on the interaction of the modes in the structure. To have a resonance, the imaginary part of the eigenvalue must be zero and the real part must be positive (and close to 1 for a large quality factor). The associated eigenvector shows the contributions of each mode that construct this specific resonance. Note that the dimension of S_u, S_d and the number of eigenvalues is equal to the number of modes to model the structure, which is typically limited to the guided modes only. The number of guided modes is indicated in Fig. 1d.

3 Q-factor and Results

For true BICs, the eigenvalue alone suffices as we just need $\lambda_{real} = 1$ and $\lambda_{imag} = 0$. For UGRs, we have losses on one side of the cell, meaning that the real part of the round-trip eigenvalue is not sufficient to characterize the resonances. To solve this, we separate the Q-factors of the top and bottom parts of the cell:

$$Q_u = \frac{2\omega_0 L}{|v_g| T_u} \quad \text{and} \quad Q_d = \frac{2\omega_0 L}{|v_g| T_d}$$

where ω_0 is the angular frequency, L is the height of the particles, v_g the (averaged) group velocity, and T_u, T_d the transmission losses of upper and lower half, respectively. The transmissions are computed via the half-trip matrices and the specific eigenvectors. Figure 2 shows the results for the array of Fig. 1. We can find the precise position of BICs and UGRs in any parameter space (here, the angular frequency vs. the height

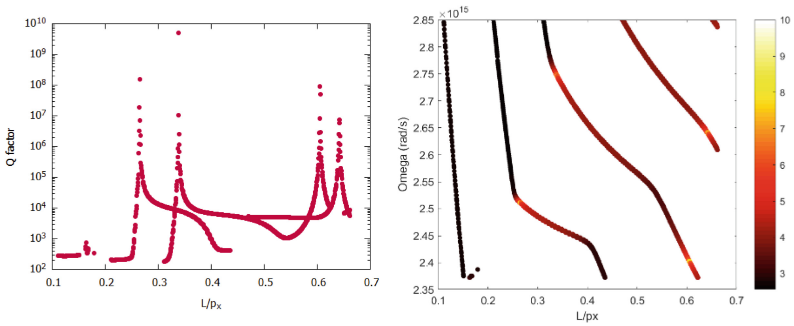

Fig. 2. (Left) The quality factor for the top and bottom sides of the structure (equal for the symmetric quasi-BIC). (Right) Placement of the resonances in the parameter space of frequency versus height (color indicates the Q-factor).

of the particles), and via the eigenvectors we obtain information e.g. about the near-field. Figure 3 shows results of the multimodal method for a structure with top-down asymmetry. We observe a good agreement between the multimodal analysis and an eigenmode solver, proving the viability of our method for high contrast UGRs.

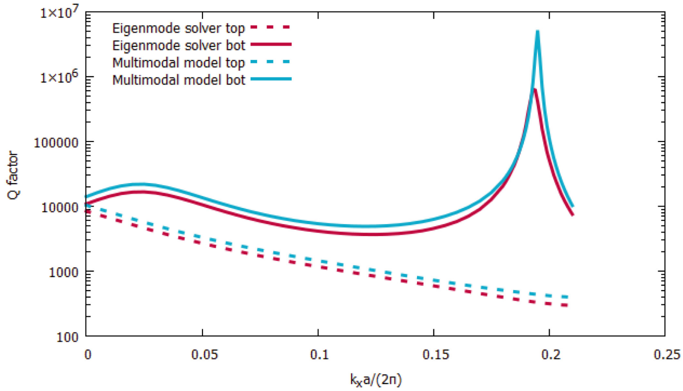

Fig. 3. Comparison of Q factors between the multimodal method and a rigorous eigenmode solver for a UGR structure.

4 Extension to 3D

The method is also useful in a 3D context. We are currently analyzing a structure used to demonstrate quasi-BICs for sensing via symmetry breaking effects [5]. We study a 2D array of cylindrical silicon particles (Fig. 4). The goal of this study is to understand how the symmetry breaking in size and position allows tuning the position of BICs. Connected with sensing experiments, we also examine the impact of different superstrate refractive indices on the resonances.

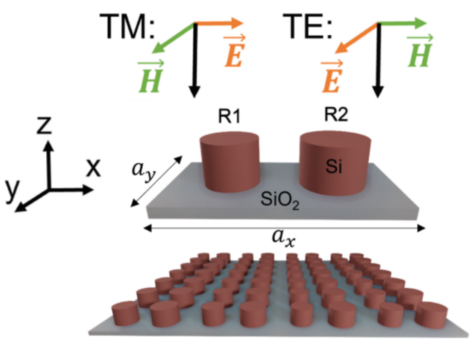

Fig. 4. Illustration of the array. a_x = *408* nm and a_y = *204* nm. The height of the particles is *90* nm. The radii are varied to tune the resonances.

We have initial results for the multimodal approach in this 3D structure. The electric field profiles obtained via the multimodal method (Fig. 5b) fit well with the results of a scattering simulation (Fig. 5a), showing that a decomposition in multiple fundamental modes can explain the resulting field in the array. The first quasi-BIC (on the left of Fig. 5) is mainly monomodal, while the second quasi-BIC (right of Fig. 5) is a composition of around 40% and 60% of 2 interacting modes. This shows that our model works for different types of BICs.

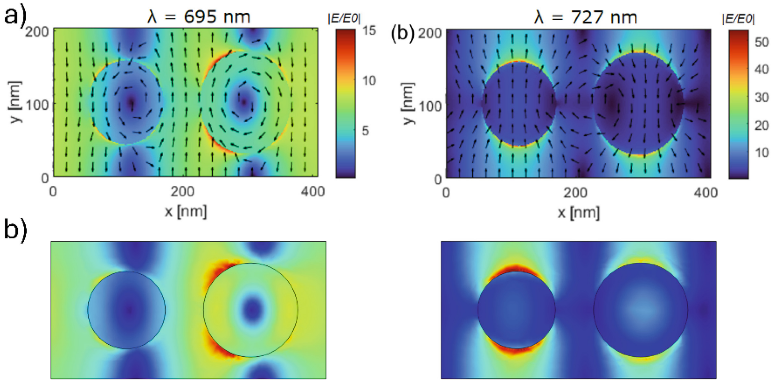

Fig. 5. Profile of the normalized norm of the electric field. a) Profile obtained by means of a scattering simulation on COMSOL. b) Profile obtained via the multimodal computation mixing waveguide simulations and analytical calculations.

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