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Polarization mixing, bound states in a continuum, and exciton-polaritons in photonic crystal slabs by a guided-mode expansion approach

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Abstract. Photonic crystal (PhC) slabs, or patterned multilayer waveguides, are known to support truly guided modes with no losses, as well as quasi-guided modes that lie in the continuum of far-field radiation. In this contribution, we present a guided-mode expansion approach – and the corresponding free software named `legume` – that allows calculating a number of features of PhC slabs: (a) symmetry properties and the issue of polarization mixing in coupling to far-field radiation; (b) the occurence of bound states in a continuum, which have infinite Q-factor and give rise to topological singularities of the far-field polarization; (c) the description of active two-dimensional layers through a suitably formulated light-matter coupling Hamiltonian, allowing to describe the regime of strong coupling leading to photonic crystal polaritons. Comparison with rigorous coupled-wave analysis, and the insurgence of non-hermitian features in the optical properties, are also addressed.

1 Introduction

Photonic crystal (PhC) slabs have been at the heart of nanophotonic research in the last three decades. They support truly guided modes that lie below the light line in the k-ω plane, and quasi-guided modes that lie above the cladding light line(s) and are subject to radiative losses. The description of both kinds of modes by the guided-mode expansion (GME) method was proposed years ago [1]. A new implementation named `legume` for general multilayer waveguides, which is compatible with automatic differentiation (AD) and allows for inverse design, was developed recently [2]. In the present work, we describe a novel version of `legume` with several new features and examples of applications. In particular, we describe symmetry properties and the issue of polarization mixing in coupling to far-field radiation, the emergence of bound states in a continuum (BICs) with diverging Q-factor, and the treatment of light-matter interaction in the presence of excitonic resonances, leading to the strong coupling regime that describes photonic crystal polaritons.

2 Method and results

The method relies on an expansion of the magnetic field in the basis of guided modes of an effective homogeneous waveguide. The second-order equation for the magnetic field is transformed into an eigenvalue equation which is solved numerically. For quasi-guided modes that lie above the cladding light line(s) in k-ω plane, coupling to leaky PhC modes is taken into account by time-dependent perturbation theory. Although GME is an approximate method, it is computationally efficient, especially for low-loss (high-Q) modes that are well described by perturbation theory. The `legume` implementation of GME has a backend to the Autograd AD library, thereby allowing efficient multiparameter optimization and inverse design [2].

The new version of `legume` implements the possibility of separating photonic modes according to symmetry with respect to a vertical $\mathbf{k}z$ reflection plane, i.e., a mirror plane that is defined by the in-plane wavevector $\mathbf{k}$ and the vertical (z) axis, such as along the Γ-X and Γ-M directions in the square lattice. Concerning far-field radiation, s-polarized (p-polarized) modes are odd (even) with respect to mirror symmetry in the incidence plane. We can now ask the following question: if a quasi-guided PhC mode is even (odd) under a reflection in a vertical mirror plane, does it couple only to p-polarized (s-polarized) radiation modes in the far field?

We decompose the imaginary part of the frequency into the contributions arising from coupling to s-polarized or p-polarized plane waves. In Fig. 1 we show $\Im(\omega)$ resolved into s- and p-polarizations, for modes that are even ($\sigma_{kz} = +1$) with respect to a vertical mirror plane. We find that $\sigma_{kz} = +1$ modes couple not only to p-polarized waves, but also to s-polarized plane waves, however this polarization mixing occurs only for high enough frequencies. Specifically, polarization mixing starts at the M-point at a dimensionless frequency $\omega a/(2\pi c) = 1/\sqrt{2} \simeq 0.71$, which corresponds to the cutoff for diffraction out of the $\mathbf{k}z$ plane. In general, a quasi-guided PhC slab mode with a given vertical parity can couple to far-field plane waves with the opposite parity, but only if these plane waves are out of the plane of incidence.

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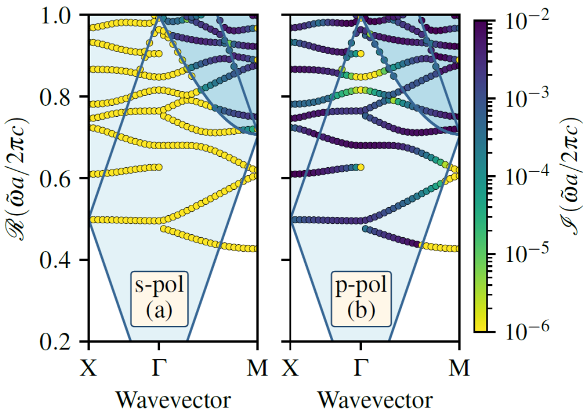

Figure 1. Dispersion and losses of even modes with respect to the mirror symmetry operator $\hat{\sigma}_{\mathbf{k}z}$, where $\mathbf{k}$ is the in-plane wavevector along the high-symmetry lines X→Γ→M. The PhC slab consists of a square lattice of period a = 400 nm, hole radius r = 100 nm, etched in a suspended slab of thickness d = 80 nm with refractive index n = 3.45.

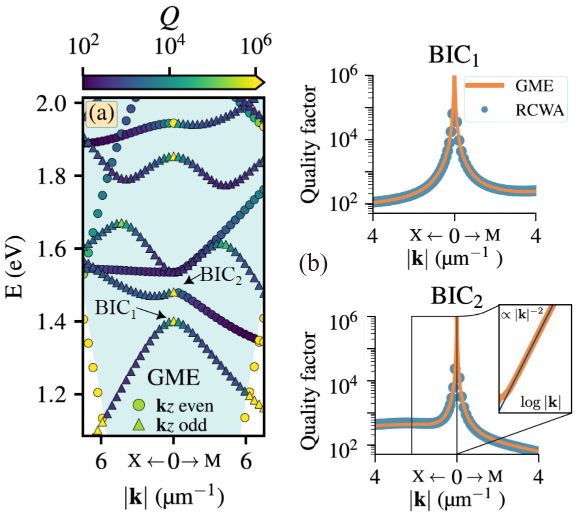

Figure 2. (a) Dispersion and losses of photonic modes, (b) Q-factor in the proximity of the two BICs indicated in (a), calculated by GME and by RCWA. Parameters are as in Fig. 1.

In Fig. 2 we show the full photonic mode dispersion in the same structure, and we highlight the behavior of the Q-factor close to two symmetry-protected BICs at $\mathbf{k} = 0$. The Q-factor diverges as $1/k^2$ for $k \to 0$, and is in very good agreement with the values calculated by rigorous coupled-wave analysis (RCWA). Topological properties of such BICs have been described elsewhere [3].

When the PhC slab contains active layers that support excitonic resonances, like quantum wells or hybrid perovskites, the 2D excitons can interact with the 2D photonic modes and enter the strong coupling regime, with the emergence of PhC polaritons. Such scenario can be treated in the `legume` code by solving the Schrödinger equation of the 2D exciton through plane-wave expansion, solving Maxwell equation for photonic modes by GME, and building up the quantum Hamiltonian that describes excitons, photons, and their mutual interaction. Such interaction depends on the excitonic parameters, in particular the oscillator strength per unit area. The second-quantized formalism is formulated in Refs. [4, 5], where is it shown that the Hamiltonian for the boson operators can be diagonalized by a Hopfield transformation. The exciton-photon coupling gives rise to characteristic anticrossings that are the fingerprints of PhC polaritons. The excitons (i.e., the matter part of the elementary excitation) inherit the symmetry properties of the excitons and also their topological features [6]. The inclusion of light-matter interaction in the `legume` code greatly expands the possibility of designing advanced photonic structure for achieving, e.g., polariton quantum fluids with desired topological properties.

3 Conclusions

The GME method in the freely available `legume` code is a powerful tool for the theoretical description of PhC slabs, including light-matter interaction via excitonic resonances, and for the direct and inverse design of advanced photonic structure. Detailed discussion is given in a forthcoming paper [7].

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